LA-UR-22-21352

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Title:	Stochastic Neutronics Primer Volume I
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Intended for:	Report
Issued:	2022-02-16

Stochastic Neutronics Primer Volume I

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Chapter 1

Introduction

The purpose of this document is to introduce the elementary concepts and to build a concrete understanding of the stochastic theory of neutron transport to the motivated undergraduate student, the Ph.D. engineer/physicist/mathematician, and the staff scientist or professor learning yet another new skill. The authors understand that there are many learning types- from visual to analytical to repetitive to word-based to analogy-based (and combinations thereof)- and so we have tasked ourselves with providing as many representations as possible within to ensure every reader a fruitful endeavor. This document is written as a set of chapters that continually build upon the previous chapter. In this chapter, we provide the discussion, motivation, and background topics for the remainder of the text.

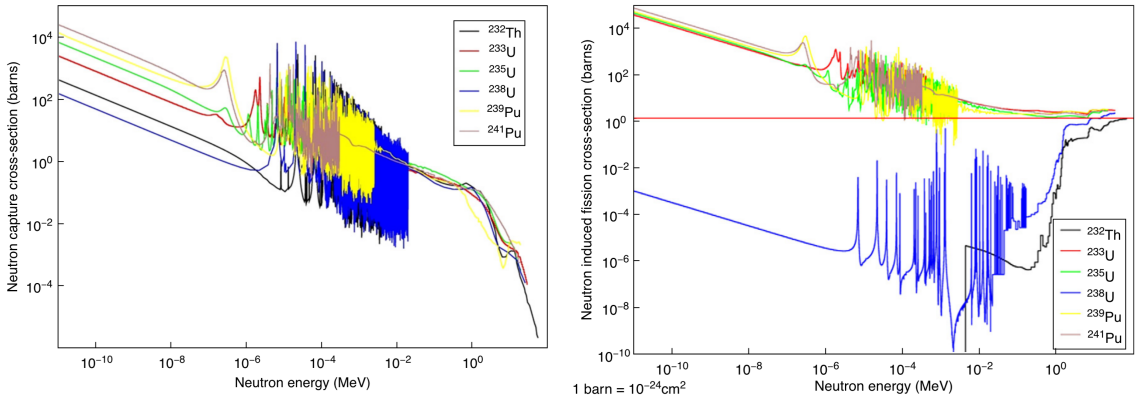
1.1 Relevant Nuclear Physics

Nuclear physics itself is a wide and rich topic and we therefore focus on the relevant fundamental concepts that we make use of in this document. We ignore spatial effects throughout the majority of this document (except in the last chapter, and only as an approximation at that) to keep clear the foundations that the field of stochastic neutronics is built upon. We are particularly interested in systems that are composed of materials that produce neutrons and are affected by neutrons that stream within them. Below, we discuss the types of interactions that a neutron may have with a medium and how we quantify those interactions by use of cross sections. This is followed by an introduction to a key element of stochasticity of a nuclear system: multiplicity distributions. We then discuss the calculation of reaction rates, which are functions of the cross sections, as well as the concept of spontaneous fission and source decay rates.

1.1.1 Neutron Interactions & Cross Sections

For the purposes of this work, we treat all neutrons as point particles, which is acceptable for higher energy neutrons for which the neutron wavelength is small enough and comparable to the size of an atom's nucleus. We may also assume that a neutron travels in a straight line until it collides with an atom because neutrons possess a neutral electric field and so they are unaffected by electric fields of atoms.

Consider now a single neutron that is moving through a medium composed of a matrix or lattice of atoms. Suppose the neutron is traveling directly towards a nucleus and therefore, from the point of view of the neutron, the nucleus appears as a solid circle that it may or may not collide with. This



(a) **(b)**

Figure 1.1: The microscopic cross sections of several isotopes for (a) capture and (b) induced fission. Plots taken from [1], data comes from the Evaluated Nuclear Data Files (ENDF) Retrieval and Plotting, Version 3.1. National Nuclear Data Center, New York, NY, October 2009.

'circle' or 'target' is of course a simplification of reality, but from this mental image we may define the *cross section* of the target nucleus as being the probability that the neutron will collide with it. More specifically in this context, we have defined the *microscopic cross section*, σ, which is measured in units of area and the most commonly used unit of measurement is the *barn*, which is equivalent to $1b = 10^{-24}cm^2$. Note that this is on the order of the cross sectional area of a representative nucleus with a radius on the order of $10^{-12}\ cm^2$.

From this, we have defined the *total microscopic cross section*, σ_t, as being the probability of simply colliding with the nucleus. There are several different mutually exclusive interactions that may occur following a collision, namely parasitic absorption (interchangeably called capture), scattering (elastic and inelastic), and induced fission which have respective cross sections σ_c, σ_s, and σ_f. Each of these is a partial cross section and their sum equals the total cross section:

$$\begin{aligned}\sigma_t(E) &= \sigma_c(E) + \sigma_s(E) + \sigma_f(E), \\ &= \sigma_a(E) + \sigma_s(E)\end{aligned} \tag{1.1}$$

where we have noted that the cross sections are functions of the incident neutron energy E and we have defined $\sigma_a(E)$ as the microscopic absorption cross section which accounts for the processes that involve the incident neutron being absorbed into the nucleus. We will discuss the fission cross section and the fission process in the next section, 1.1.2. Microscopic cross sections may be derived from experimentation or from quantum mechanical theory, and their values may vary substantially depending on the incoming neutron's energy. The cross sections are also dependent on the temperature of the medium because, as a material heats up, the nuclei gain kinetic energy and vibrate with greater frequency and amplitude; thus, one expects the sharp peaks to widen over neutron energy ranges and this is known as Doppler Broadening. Figure 1.1a shows the microscopic capture cross section for several isotopes commonly found in nuclear reactors and Fig. 1.1b shows the induced fission cross sections for the same isotopes. As we can see, the cross sections vary wildly over several orders of magnitude in both the value of the cross section and the incident neutron energy. The reason for the rapid variations and oscillations of σ for relatively small changes in neutron energy is due to wave-mechanical effects of the neutron as it penetrates the complicated

structure of the nucleus. There are plenty of sources for explaining this phenomena [2, 3], but such a discussion is beyond our present needs.

Aside from revealing some interesting nuclear properties of an isotope, the microscopic cross section may be used to determine the *macroscopic cross section* for interaction type x, Σ_x, where $x = \{t, c, s, f\}$ for the total, capture, scatter, and fission interactions. Noting that the microscopic cross section was defined for a single neutron incident on a single nucleus, we are more often concerned with a neutron traveling through a lattice of nuclei with density N atoms per volume[1]. From this, we define the *number density*, N, of the medium which may be calculated as:

$$N(t) = \frac{\rho(t) N_A}{M} \tag{1.2}$$

where $\rho(t)$ is the time-dependent density of the material $[g/cm^3]$, N_A is Avogadro's constant ($= 6.022 \cdot 10^{23} 1/mol$), and M is the molar mass of the atoms $[g/mol]$. From Eq. 1.2, we can define the macroscopic cross section for interaction x as:

$$\Sigma_x(E, t) = N(t)\sigma_x(E) \tag{1.3}$$

from which the total macroscopic cross section is defined as

$$\begin{aligned} \Sigma_t(E, t) &= \Sigma_c(E, t) + \Sigma_s(E, t) + \Sigma_f(E, t) \\ &= N(t)\big[\sigma_c(E) + \sigma_s(E) + \sigma_f(E)\big]. \end{aligned} \tag{1.4}$$

The macroscopic cross section should be thought of as the probability of colliding per unit of length travelled by the neutron resulting in interaction x. The above discussion assumes the medium is composed of a single isotope, but it is possible to determine the number density of a mixture, which can be found in [4, 5].

1.1.2 Fission & Multiplicity Distributions

As we briefly mentioned above, a neutron that collides with a nucleus may cause a fission (i.e., induce a fission) with probability σ_f. Figure 1.2 illustrates an induced fission event with the related time scales (in seconds) that show at what point in the process certain particles emerge. As we see, an induced fission initiates when a neutron collides with a nucleus, gets absorbed within the nucleus and causes it to become excited and unstable. The excited unstable nucleus then deforms and scissions into two fragment nuclei within 10^{-21} to 10^{-19} seconds[2]. These fission fragments then promptly emit neutrons within 10^{-18} seconds. Shortly thereafter, the fission fragments emit gamma rays to further de-excite (anywhere between 10^{-14} and 10^{-7} seconds) and some of these fragments will much later (relatively speaking) further decay via beta decay[3]. Not shown in the beta decay process are the additional particles that are typically emitted, such as gamma rays, beta particles, neutrinos, and antineutrinos. We focus on the neutrons that are promptly emitted as they are produced essentially simultaneously whence the excited nucleus splits. Additionally, the decay

[1] This leads into the real-world problem of analyzing many neutrons, i.e. a neutron flux, moving through many lattice atoms. We will not use the concept of the flux in this document because we are interested in probabilistic behavior of the population, whereas the flux is an average quantity.

[2] The nucleus does not split evenly into equal fission fragments but will instead result in one fragment being considerably lighter than the other. Typically, the fission product atomic numbers are concentrated in the ranges from about 80 to 105 and from about 130 to 150 in thermal reactors.

[3] Beta Minus Decay is the process of a neutron in the nucleus emitting an electron, called the beta particle, and an antineutrino which transitions the neutron to a proton. Conversely, Beta Plus Decay is the emission of a positron and neutrino which converts the proton to a neutron.

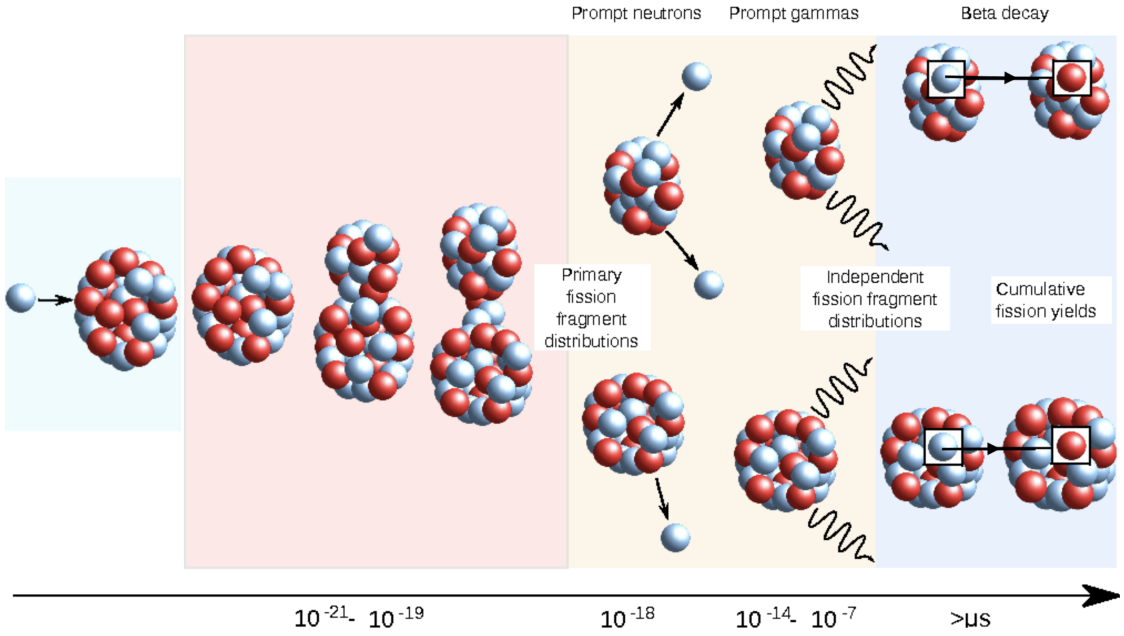
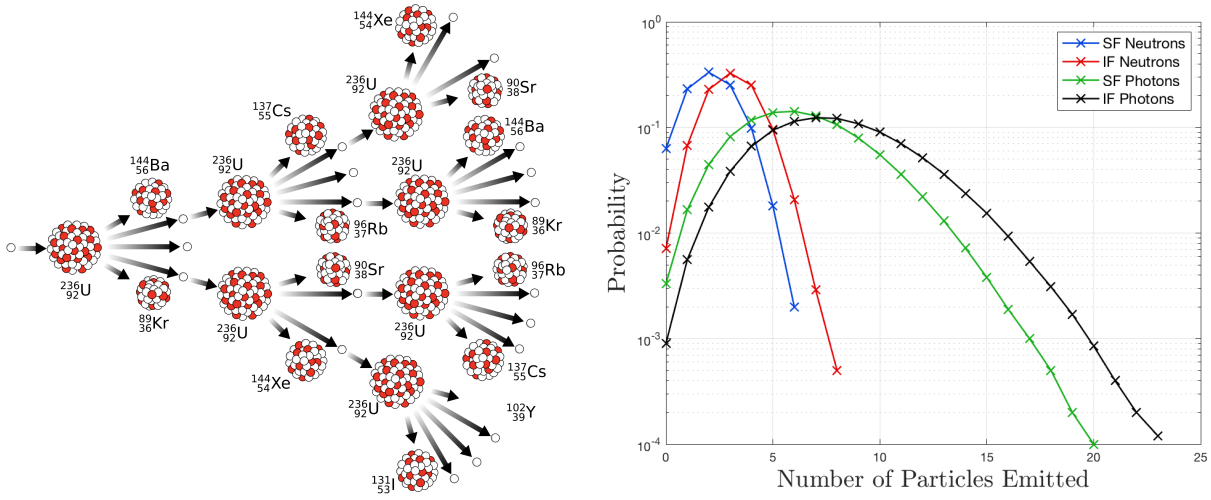


Figure 1.2: Illustration of an induced fission event with relative time scales (seconds) of the evolution of the process. Taken from www.fuw.edu and edited by P. O'Rourke.



(a) **(b)**

Figure 1.3: (a) Shows an example of a sustained fission chain and (b) shows several particle multiplicity distributions for a Pu system. ((a) was taken from MikeRun under license CC BY-SA 4.0).

of certain fission fragments will produce another neutron, called a delayed neutron which appear between microseconds to seconds after the fission event. We will ignore effects of delayed neutrons in this document and consider only the prompt neutrons.

There is another type of fission that occurs and it does so randomly and spontaneously. We therefore refer to this process as spontaneous fission (SF) and it is the radioactive decay process of an unstable nucleus randomly splitting into two fission fragments and emitting neutrons as well as other particles. The SF process does not require a neutron for it to happen and therefore nothing can induce it except for nuclear instability and time. We will treat the SF process as a source within this work because it indiscriminately adds neutrons to the system.

In the event of either an induced fission or a spontaneous fission, neutrons are emitted which may then go on to induce more fissions. This process is illustrated in Fig. 1.3a, where we see a single neutron has the potential of starting many fission reactions within the system. This chain of fission events is called a *fission chain* reaction and is the basis for the design of nuclear reactor power plants for the production of electricity. One of our main focuses in this document is to model and predict the behavior of fission chains from a probabilistic point of view.

An additional feature of the induced fission and spontaneous fission processes are the random number of particles that may emerge from those events (this feature is hinted at in Fig. 1.3a where we see some fission events result in 2 neutrons while others result in 3). We define q_ν^x as being the probability that ν particles are emitted following event type x, where $x = \{f, S\}$ for induced fission and spontaneous fission, respectively. The collection of these probabilities is called the *multiplicity probability distribution*, or simply the multiplicity distribution. As an example, Fig. 1.3b shows the neutron and photon multiplicity distributions for induced fission (IF) and spontaneous fission (SF) for a 20 wt% ^{240}Pu and 80 wt% ^{239}Pu system [6]. We can see that the number of neutrons emerging from a fission event may range from zero up to some max number, ν_m^x, typically between 6 and 8. Each of these emission numbers has the associated probability q_ν^x and the distribution is normalized as

$$\sum_{\nu=0}^{\nu_m^x} q_\nu^x = 1. \tag{1.5}$$

In this document, we consider only the neutron multiplicity distribution, but show the photons to help the reader to understand that this is a characteristic of any fission process and the particles resulting thereof (another random outcome from a fission is the masses of the fission fragments, which ultimately dictates the remaining decay chain and resulting particles). Typically, we deal with the average number of neutrons that are emitted from fission event type x, $\overline{\nu}_x$, which is calculated as:

$$\overline{\nu}_x = \sum_{\nu=0}^{\nu_m^x} \nu q_\nu^x. \tag{1.6}$$

This is the quantity one uses when analyzing the neutron transport equation and/or the neutron diffusion equation when induced fission is included.

We finish this section by discussing the concept of neutron multiplication due to the induced fission process. As we now know, in certain materials a single neutron may induce a fission which will bring forth an average of $\overline{\nu}_f$ neutrons per fission. Those neutrons, the progeny of the first neutron, will continue on and may induce other fissions. Each time a set of neutrons induces another fission and creates new neutrons, a new generation of neutrons is born. We may quantify the behavior of the neutron population over many generations using the multiplication factor, k, which is defined as

$$k = \overline{\nu}_f \frac{\Sigma_f}{\Sigma_a}, \tag{1.7}$$

where $\Sigma_a = \Sigma_f + \Sigma_c$ is the macroscopic absorption cross section. If $k < 1$, the fission chain will eventually extinguish and the system is considered subcritical. If $k \equiv 1$, the fission chain will propagate forever and the system is exactly critical. For $k > 1$, the chain will grow unbounded and the system is supercritical. We note that the ratio of the cross sections Σ_x/Σ_a is the probability that, upon a neutron colliding with a nucleus, event x will occur and we write this as:

$$p_x = \frac{\Sigma_x}{\Sigma_a}. \tag{1.8}$$

1.1.3 Reaction & Source Decay Rates

In the proceeding chapters, we must concern ourselves with the rates at which neutrons are interacting with the medium and, if a source is present, we must know the rate at which that source is spontaneously decaying and emitting neutrons into the system. These rates, referred to as *reaction rates* for neutron interactions and simply the *source strength*, help to characterize how the system will evolve in time and prove quite useful for that reason.

The primary interactions to consider are those that remove neutrons from or introduce neutrons to the system at a given energy E; these mutually exclusive events are capture, scattering, induced fission, and spontaneous fission (there is also the loss mechanism due to leakage which is a function of the system's geometry, but we will ignore that for now). The system may be characterized by the reaction rates, $\lambda_x(E,t)$, defined as the probability per neutron per unit energy per unit time that the particular event x will occur, and a source strength, $S(E,t)$, defined as the probability that a source event will occur per unit energy per unit time. The reaction rates at a given time, t, may be calculated using the macroscopic cross section for reaction x and the neutron speed, $v(E)$, as

$$\lambda_x(E,t) = v(E)\Sigma_x(E,t), \tag{1.9}$$

where we will use the subscripts $x = \{c, f\}$ for capture and induced fission. We note that the absorption reaction rate is the sum of the capture and induced fission rates and the total reaction rate is then the absorption added with the scattering rate:

$$\lambda_a(E,t) = \lambda_c(E,t) + \lambda_f(E,t) \tag{1.10a}$$

$$\lambda_t(E,t) = \lambda_a(E,t) + \lambda_s(E,t) \tag{1.10b}$$

$$\tau(E,t) = \frac{1}{\lambda_t(E,t)}, \tag{1.10c}$$

where we have introduced $\tau(E,t)$ as the average lifetime of a neutron with energy E at time t. We may also include a generic loss rate due to leakage, $\lambda_\ell(E,t)$, which could be contributed to $\lambda_t(E,t)$ by simply adding it.

We may also calculate the intrinsic source strength for a given system with mass m which may be composed of any number of isotopes that may undergo radioactive decay using the formula

$$S(E,t) = m(t)N_A \sum_i \frac{p_{sp,i}(E)\lambda_i w_i}{M_i}, \tag{1.11}$$

where N_A is Avogadro's Constant, $p_{sp,i}$ is the probability that a radioactive decay of isotope i is a spontaneous fission event and emits a neutron of energy E, λ_i is the radioactive decay constant, w_i is i's weight fraction, and M_i is the molar mass.

1.2 What are Master Equations?

Historically, a master equation is called as such[4] because it acts as an umbrella equation within the hierarchy of equations encountered in mathematical physics from which many properties of the model may be derived- thus, the equation is 'ruling' over the subsequent equations. At its core, a master equation is simply an equation whose solution is a probability distribution function (PDF) which describes a discrete-state continuous-time Markov process[5]. This equation could be an ordinary differential equation (ODE), partial differential equation (PDE), integro-differential equation (IDE), and so on. In this document, we will be working with master equations that are ODEs and PDEs, but in later volumes we will see master equations of the IDE variety. Master equations are used in quantum mechanics, stochastic chemical kinetics, gene regulatory networks, disease propagation, evolutionary game theory, social and economic processes, queuing processes, traffic jam modeling, boson condensation, and many others [13]. We also note that the master equation counterpart for which the solution is a probability density function (which is used for a continuous-state continuous-time Markov process) is the Fokker-Planck equation. Let us now build up our understanding of the nomenclature we will see throughout this document and how to interpret it.

We begin by asking the broad question we want to answer, "what is the probability that a system initially in state m at time t_o is then in state n at a later time t?" The answer to this question is symbolized by the quantity $P_{n|m}(t|t_o)$ and should be read as, "the probability of being in state n at time t conditioned on the system having been in state m at an earlier time t_o." The "$n|m$" symbolizes conditions, where the earlier conditions are always on the right and the resultant state and time is on the left.

In a general sense, $P_{n|m}(t|t_o)$ can be calculated by summing all the possible states the system may occupy on its path from state m at t_o to state n at t. Since we are beginning in state m at t_o, we need to consider the probability that the system will transition to state i at some time t', where $t' \in [t_o, t]$, and then multiply this quantity by the probability of transitioning from state i at t' to state n at t. This can be written mathematically as

$$P_{n|m}(t|t_o) = \sum_i P_{n|i}(t|t')P_{i|m}(t'|t_o). \tag{1.12}$$

To reiterate, Eq. 1.12 defines the probability $P_{n|m}(t|t_o)$ as being equivalent to the sum of all probabilistic pathways the system may travel upon as it transitions from the initial state to the final state. The states "i" are referred to as *intermediary states* later in this primer. In this current general form, this equation is referred to as the Chapman-Kolmogorov Equation that describes a discrete-state continuous-time Markov process [8, 11]. As a tip, we suggest reading each term on the RHS starting from the most-right factor and moving left as this coincides with the chronology of the events (i.e., read $P_{i|m}(t'|t_o)$ first, then $P_{n|i}(t|t')$).

From the Chapman-Kolmogorov equation 1.12, our first task will be to define the intermediary state time t'. The two most common locations to define where t' occurs within the problem's time domain are either immediately following the initial time or just before the final time. Figure 1.4 shows these two options for us, where we have explicitly defined t' as a function of either the initial/injection time or the final time as well as an arbitrarily small time interval Δt. We assume

[4]The name "master equation" was originally coined by Nordsieck, Lamb, and Uhlenbeck in their study of the Furry model of cosmic rain showers [13].

[5]A Markov process refers to the memorylessness of the particles such that the current state of the system is only a direct result of the most recent state of the system. As an example, imagine a neutron with energy, E- that neutron may have obtained E from scattering off a nucleus or may have emerged from fission with E. In either case, it is E that dictates the possible next steps for the neutron rather than its process of origin.

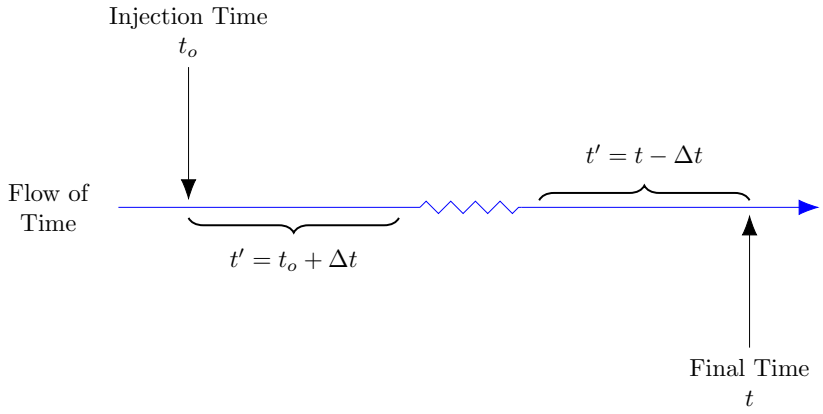


Figure 1.4: Time variables used for the forward and backward formulation.

Δt is small enough that effectively only a single event may occur (as in, only a single state-transition may occur). Selecting one definition of t' over the other will result in different forms of the master equation that we will become quite familiar with by the end of this primer. The two selection methods are called the Forward Formulation (FF) for t' near the final time and the Backward Formulation (BF) for t' near the beginning:

$$\begin{cases} \text{Forward:} \quad t' = t - \Delta t \\ \text{Backward: } t' = t_o + \Delta t. \end{cases} \tag{1.13}$$

From this, it is clear that the Chapman-Kolmogorov equation is essentially a probability balance and, by selecting t', we are conducting the probability balance in either the *last collision interval* in the Forward Formulation or in the *first collision interval* in the Backward Formulation. Recall that we are forcing Δt to be arbitrarily small to the point that, if an event occurs that transitions the system to a new state, no other event may conceivably occur. Thus, a collision interval should be regarded as the amount of time that it takes for a collision to take place (which we have shown in Fig. 1.2, is on the order of 10^{-20} s).

By selecting either the FF or BF, we must then determine the transitions that may occur in the collision interval of choice. A transition from one state to another can be quantified by using transfer probability rates or, as we have defined them, reaction rates λ from Sec. 1.1.3. Recalling that λ_x is the probability per neutron per unit time that event x will occur, we may then determine the transition probabilities of Eq. 1.12. Thus, to get a probability from the reaction rates we simply multiply by the time interval Δt, i.e. $\lambda_x \Delta t =$ the probability of event x occurring per neutron in the time span Δt. Going back to a more general mathematical notation, we will write our reaction rates as transfer rates: $\lambda_{j \leftarrow i}$, meaning the probability per unit time that an event occurs which transfers the system from state i to state j. We need to be cautious about the transfer rates because they will appear differently depending on the FF versus BF. In the forward approach, we are taking t' in the last collision interval and thus we need to consider transfer rates that take the system from state i to state n. In the backward approach, we are taking t' in the first collision interval and thus need to consider transfers from state m to state i. This gives the Chapman-Kolmogorov equation a

new form:

$$\text{F:} \quad P_{n|m}(t|t_o) = \sum_i \lambda_{n\leftarrow i}\Delta t P_{i|m}(t-\Delta t|t_o) \tag{1.14a}$$

$$\text{B:} \quad P_{n|m}(t|t_o) = \sum_i P_{n|i}(t|t_o+\Delta t)\lambda_{i\leftarrow m}\Delta t. \tag{1.14b}$$

Let us now read the RHS of each equation to better understand how the FF and BF changed our view of the problem. It is important to keep in mind that the LHS did not change and thus the two methods provide the same answer, we will see this proved many times throughout this primer. The forward RHS is read as, "the probability of being in state i at $t-\Delta t$ conditioned on being in state m at t_o times the probability of then transferring from state i to state n in the time interval Δt leading to time t." The backward RHS is read as, "the probability of transferring from the initial state m to state i in the time interval $[t_o, t_o+\Delta t]$ times the probability of being in state n at t conditioned on being in state i at $t_o+\Delta t$." Equations 1.14 are referred to as the Forward Chapman-Kolmogorov equation and the Backward Chapman-Kolmogorov equation, respectively.

Before deriving the forward and backward master equations, there is one more transfer probability that we must consider: the probability of self-transfer $\lambda_{n\leftarrow n}\Delta t$. First, we note that the quantities $\lambda_{n\leftarrow i}\Delta t$ are probabilities and are therefore normalized:

$$\sum_i \lambda_{n\leftarrow i}\Delta t = 1. \tag{1.15}$$

From this, we may define the probability of self-transfer as

$$\lambda_{n\leftarrow n}\Delta t = 1 - \sum_{i\neq n}\lambda_{n\leftarrow i}\Delta t. \tag{1.16}$$

The above relates to the FF, but the same holds for the BF for which one would write:

$$\lambda_{m\leftarrow m}\Delta t = 1 - \sum_{i\neq m}\lambda_{i\leftarrow m}\Delta t. \tag{1.17}$$

In a physical setting, the self-transfer probability refers to the probability of no event occurring in Δt. Knowledge of this scenario is important as it is connected to the probability that the system is already in state n.

We have all the ingredients to derive the master equations and we start by separating the self-transfer probabilities from the respective Chapman-Kolmogorov equations:

$$\text{F:} \quad P_{n|m}(t|t_o) = \sum_{i\neq n}\lambda_{n\leftarrow i}\Delta t P_{i|m}(t-\Delta t|t_o) + \lambda_{n\leftarrow n}\Delta t P_{n|m}(t-\Delta t|t_o) \tag{1.18a}$$

$$\text{B:} \quad P_{n|m}(t|t_o) = \sum_{i\neq m} P_{n|i}(t|t_o+\Delta t)\lambda_{i\leftarrow m}\Delta t + P_{n|m}(t|t_o+\Delta t)\lambda_{m\leftarrow m}\Delta t. \tag{1.18b}$$

Now using Eqs. 1.16 and 1.17, we have:

$$\text{F:} \quad P_{n|m}(t|t_o) = \sum_{i\neq n}\lambda_{n\leftarrow i}\Delta t P_{i|m}(t-\Delta t|t_o) + \left[1 - \sum_{i\neq n}\lambda_{n\leftarrow i}\Delta t\right] P_{n|m}(t-\Delta t|t_o) \tag{1.19a}$$

$$\text{B:} \quad P_{n|m}(t|t_o) = \sum_{i\neq m} P_{n|i}(t|t_o+\Delta t)\lambda_{i\leftarrow m}\Delta t + P_{n|m}(t|t_o+\Delta t)\left[1 - \sum_{i\neq m}\lambda_{i\leftarrow m}\Delta t\right]. \tag{1.19b}$$

We next rearrange the above equations to find:

$$\text{F:} \quad \frac{P_{n|m}(t|t_o) - P_{n|m}(t-\Delta t|t_o)}{\Delta t} = -P_{n|m}(t-\Delta t|t_o)\sum_{i\neq n}\lambda_{n\leftarrow i} + \sum_{i\neq n}\lambda_{n\leftarrow i}P_{i|m}(t-\Delta t|t_o) \tag{1.20a}$$

$$\text{B:} \quad \frac{P_{n|m}(t|t_o) - P_{n|m}(t|t_o+\Delta t)}{\Delta t} = -P_{n|m}(t|t_o+\Delta t)\sum_{i\neq m}\lambda_{i\leftarrow m} + \sum_{i\neq m}P_{n|i}(t|t_o+\Delta t)\lambda_{i\leftarrow m}. \tag{1.20b}$$

Finally, we convert the above equations into differential equations, in fact they are classified as differential-difference equations because the solutions are coupled via a discrete index. This conversion is done by taking the limit as $\Delta t \to 0$ and recalling the limit definition of a derivative to arrive at the forward and backward master equations:

$$\text{F:} \quad \frac{\mathrm{d}P_{n|m}(t|t_o)}{\mathrm{d}t} = -P_{n|m}(t|t_o)\sum_{i\neq n}\lambda_{n\leftarrow i} + \sum_{i\neq n}\lambda_{n\leftarrow i}P_{i|m}(t|t_o) \tag{1.21a}$$

$$\text{B:} \quad -\frac{\mathrm{d}P_{n|m}(t|t_o)}{\mathrm{d}t_o} = -P_{n|m}(t|t_o)\sum_{i\neq m}\lambda_{i\leftarrow m} + \sum_{i\neq m}P_{n|i}(t|t_o)\lambda_{i\leftarrow m}. \tag{1.21b}$$

There are several striking differences between these two master equations. First, we see that the backward master equation (BME) has a negative time derivative which indicates that time is actually reversed (which is somewhat non-intuitive, but we will see it makes sense in action later). Another quirk of the BME is that the derivative is taken with respect to the initial time and not the final time. We call the time that is being differentiated the *operating time* as it is the time that is variable. In that sense, the BME has a "final" condition rather than a typical initial condition because the final time is held constant. We will see that, unlike the BME, the forward master equation (FME) is treated like a typical ODE with an initial condition that dictates the evolution of the probabilistic state of the system. For that reason, it is cumbersome and unnecessary to continue to carry around the conditional statements on the FME solution and we may simplify the notation slightly as:

$$\text{F:} \quad \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = -P_n(t)\sum_{i\neq n}\lambda_{n\leftarrow i} + \sum_{i\neq n}\lambda_{n\leftarrow i}P_i(t). \tag{1.22}$$

There will be a notational simplification for the BME as well (we will be able to drop the m, but not t_o since it is the operating time), but we leave it as is for now. Such types of variables that do not provide the necessary information about an equation are called *nuisance variables* [14].

From this demonstration, we have seen that the Chapman-Kolmogorov equation can be viewed as a probability balance conducted either in the first or last collision interval. From this balance, we were able to rearrange the equation with some simple algebraic manipulations and then convert the equation into a linear first-order differential-difference equation known as a master equation. Solving either forward or backward master equation will provide the same answer and, in the 0-D setting, the choice of which to use is entirely up to the researcher's preference. We will see in a later volume that the BF proves superior when spatial, angular, etc. dependence are included (so it does not hurt to learn it now). Given the model at hand, the master equation might be solved easily and outright, or it might not have a solution at all. In this primer, we will apply a solution algorithm that is used for the most complicated of master equations (think energy, space, angle dependence, and so on) and we therefore show how to apply it to solve the simple master equations and to gain an intuition of the implications/limits of the approximations we use. This solution algorithm is introduced next.

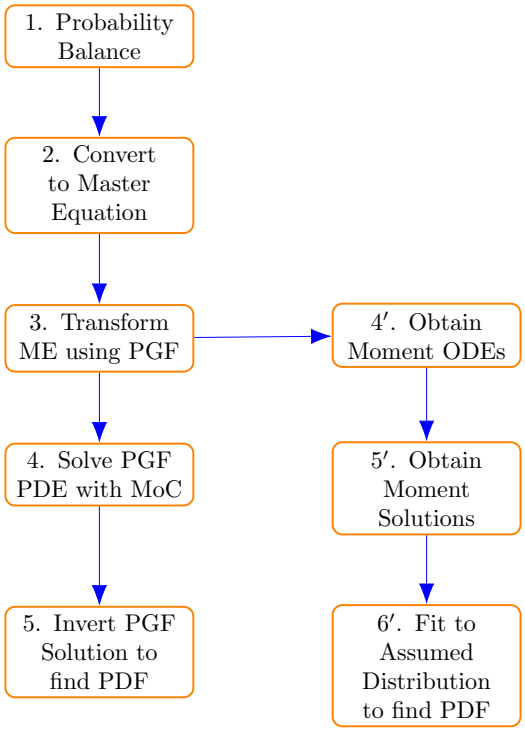


Figure 1.5: The Master Equation Solution Algorithm (MESA).

1.3 The Master Equation Solution Algorithm

The process of analytically solving Master equations, both forward and backward, can be summarized in a handful of straightforward mathematical steps. It is this algorithm that we wish to convey to the reader so they are capable of deriving, solving, and analyzing their own master equations. Figure 1.5 illustrates the Master Equation Solution Algorithm (MESA) that we will be using throughout every chapter in this primer. We believe it is most instructive to introduce this subject using the relevant neutron transport language, as it is the subject of this work, but this algorithm may easily be applied to all of the disciplines and general master equations mentioned in Sec. 1.2.

Focusing on Fig. 1.5, the left column concerns the process for obtaining exact or approximate analytical solutions to the Master equation itself and we will refer to it as the Analytical MESA (AMESA). The right column that splits at step 3 is used more commonly for obtaining the solution using numerical methods and we will refer to it as the Numerical MESA (NMESA). The focus of this primer is to utilize AMESA to obtain exact closed-form analytical solutions to the FME and BME, and we will discuss the NMESA in the very last chapter to demonstrate its utility as it will be used in later primer volumes.

For us, the analytical solution to the master equation, $P_{n|m}(t|t_o)$, will be obtained via the AMESA. For step 1, we conduct a probability balance either in the first collision interval or last collision interval (note any of the progressive Chapman-Kolmogorov equations 1.12, 1.14, 1.18, 1.19). The balance equation will define all the physical processes and their effects we want to include in the

final solution[6]. In step 2, we then convert the balance equation to a master equation by rearranging and taking the limit as the collision interval becomes instantaneous (recall Eqs. 1.20 and 1.21). Step 2 is as far as Sec. 1.2 got us, and we state the remaining steps below and summarize thereafter.

- Outline of AMESA:
    1. Conduct probability balance,
    2. convert to a master equation (ME),
    3. transform ME to a PDE using probability generating function (PGF), $G(z, t|t_o)$,
    4. solve PGF PDE with Method of Characteristics (MoC),
    5. invert $G(z, t|t_o)$ solution to obtain number distribution, $P_{n|m}(t|t_o)$.

For step 3, we are tasked with transforming the master equation to a partial differential equation (PDE) using the probability generating function (PGF), symbolized as $G(z, t|t_o)$. The PGF is treated as a discrete transform (if you have dealt with Laplace transforms or Fourier transforms, those are continuous transforms) that transforms the master equation from discrete n space to a continuous transform space with transform variable z. We will not explicitly define the PGF here, but it suffices to mention that the PGF effectively consolidates the infinite number of coupled ODEs of the master equation (there are an infinite number because $n = 0, 1, 2, \ldots, \infty$) into a single PDE. This makes the problem a little more tractable, with the trade-off being the reduction to a single equation but that equation is a PDE.

Step 4 is typically where the bulk of the work is done. The PGF PDE, in the 0-D setting, turns out to be linear hyperbolic PDE which can be solved (or partially solved) using the Method of Characteristics (MoC). We will become familiar with the MoC, but the gist is to convert the PDE to a system of ODEs which can be solved to find the full solution. Once we have the full solution, $G(z, t|t_o)$, we then convert back from z space to n space in step 5. In performing all these steps, we should emerge with an analytical solution!

It is true that many, if not most, master equations will not have a closed-form analytical solution, but there are other options one has in elucidating vital information about the probabilistic behavior of the system under study. In particular, we may use the additional branch of the MESA of Fig. 1.5, the NMESA, to obtain equations for the moments of the distribution function which are useful in their own right, but can also be used to fit distributions to find approximate, if not exact, solutions to the master equation. The outline of NMESA is as follows:

- Outline of NMESA:
    1. Conduct probability balance,
    2. convert to a master equation,
    3. transform using PGF,
    4′. derive equations for the moments,
    5′. solve the moment equations (either analytically or numerically),
    6′. and fit a distribution using the moments.

[6]Often times, approximations will need to be made or certain physical effects will need to be ignored in order to get a final solution, we will see this several times in this work. Case-in-point, this work ignores spatial effects entirely.

There is a convenient identity that we may apply to the PGF to obtain the moments of the distribution we seek (e.g., the mean, variance, skewness, and so on), which step $4'$ refers to. We will see this identity used in practice in the final chapter of this primer. These moment equations are typically coupled ODEs that can sometimes be solved analytically, but are more likely to be solved numerically. As a sneak-peak, we will see that the ODE for the first moment is the well-known point kinetics equations (recall, the master equation is ruling over the lower-information equations!) Upon solving for the moments in step $5'$, we then need to assume a form of the distribution for which we may then use the moments to construct the distribution. The moments themselves provide useful information about the profile and characteristics of the distribution and the fitted distribution itself (which is more than likely an approximate solution) provides the desired quantity we seek.

Although we did not mathematically define some of the quantities we have discussed in this section (e.g., the PGF, moment identities), we hope to have conveyed the principle motivations for using the MESA and when and how to use the AMESA or the NMESA. We will apply this algorithm every time we encounter a master equation in this primer.

Chapter 2

Radioactive Decay Model

In this chapter, we begin our journey into formulating, solving, and utilizing Master equations to better understand nuclear phenomena. We shall begin with a simple radioactive decay model to utilize the formal mathematical process outlined in Chapter 1 Sec. 1.3. We commence the expedition by introducing what is known as the Forward Master Equation (FME) Formulation in Sec. 2.2 followed by the Backward Master Equation (BME) Formulation in Sec. 2.3. The primary difference between the two formulations is in how one conducts the probability balance, but it is important to note that the resulting solutions (the number distributions) are the same and it is therefore the scientist's preference as to which formulation they use in the 0-D setting.[1] In Sec. 2.1, we introduce the concepts and assumptions made that apply to both the forward and backward Master equation formulations to reduce redundancy. In both Secs. 2.2 and 2.3, we go through the step-by-step process for formulating and solving Master equations that was outlined in Sec. 1.3.

2.1 The Model

Suppose we are observing a system with a neutron source that constantly, randomly, and spontaneously decays. Following is a list containing the primary assumptions we use in the forward and backward master equation formulations:

- the system is large enough that we do not need to take spatial effects into account,
- the source is uniformly distributed throughout the system and we quantify the source magnitude, S, using Eq. 1.11 (S is defined as "the probability of a source event occurring per unit time" and thus S is a probability density function),
- after a source event occurs, a single neutron is emitted traveling with speed v,
- the medium is neutron-transparent, i.e., there are no neutron interactions and thus a neutron simply travels indefinitely once it appears following a source event,
- that there are 0 neutrons within the system for times before $t = t_o$.

[1] We will see in a later volume that the backward formulation is indeed the superior of the two formulations when we account for space, energy, and angular dependence.

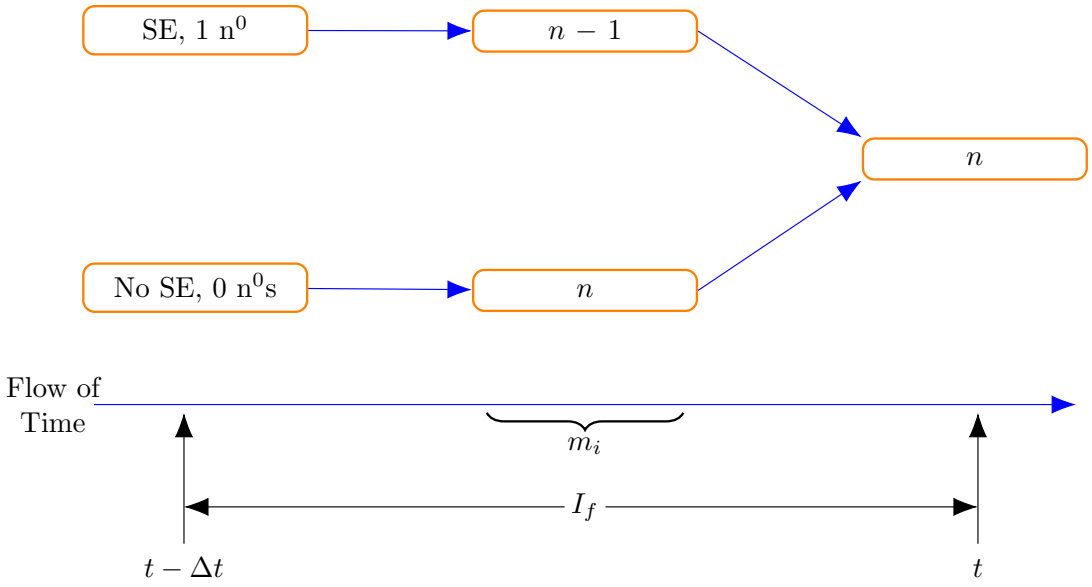


Figure 2.1: Mutually exclusive events that may occur in time interval I_f with their associated states, m_i, for a singlet-emitting source in a neutron-transparent medium. SE = Source Event. Either a SE occurs in I_f, producing 1 n^0, or no SE occurs and there must already be n n^{0}s at the beginning of I_f.

2.2 Forward Formulation

The forward formulation is outlined below, following the step-by-step rules of the master equation solution algorithm described in Sec. 1.3.

2.2.1 Probability Balance & Master Equation

We begin by defining the probabilistic quantity we wish to obtain:

$$P_n(t) = \text{the probability of there existing } n \text{ neutrons within the system at time } t \text{ due to the introduction of a source of strength } S \text{ at an earlier time } t = t_o.^2 \tag{2.1}$$

To determine $P_n(t)$, we use knowledge of the possible states the system could be occupying a short time before t given by $t - \Delta t$. Thus we will conduct a probability balance over the time domain:

$$I_f = [t - \Delta t, t], \tag{2.2}$$

where the subscript f refers to this being the forward time interval (as opposed to the backward time interval we will see in Sec. 2.3). We assume Δt is sufficiently small enough that only a single source

[2]Throughout this chapter, one could equivalently interpret n as the total number of source events that have occurred or as the total neutron population. Interpretation of n as the total number of source events gives rise to the namesake of this chapter. However, because we wish to convey the formulation process in terms of neutron populations within this primer, we will be referring to n as the total neutron population in this chapter. This ambiguity of n is lost once we allow for neutron interactions, or if we allow for more than one neutron to be emitted per source event.

event may reasonably occur within it. In constructing the probability balance using the forward formulation, let us first state the possible events that may occur within the short time interval I_f:

1. No source event occurs
2. A source event occurs, producing 1 neutron.

Only these two events may occur because we are not allowing for neutron interactions, in later chapter this list will grow. To further illustrate the events that may occur leading up to time t, we provide an event tree in Fig. 2.1, where SE stands for source event. In the figure, we see the event that may occur in the far-left bubbles with the resultant number of neutrons (symbolized by n^0, in-line with standard model notation) that emerge, followed by the intermediary state m_i- the i^{th} state that is event-connected to state n- which we use to aid in the forthcoming probability balance. Again, this event tree will grow as more physics is incorporated in later chapters. Using the list above, we may write the probability balance in words as follows:

$$\begin{aligned} P_n(t) = &\left(\begin{array}{l} \text{Probability of no source} \\ \text{event occurring in } I_f \end{array} \right) \times \left(\begin{array}{l} \text{Probability of being in} \\ \text{state } n \text{ at time } t - \Delta t \end{array} \right) \\ &+ \left(\begin{array}{l} \text{Probability of 1 source} \\ \text{event occurring in } I_f \end{array} \right) \times \left(\begin{array}{l} \text{Probability of being in a} \\ \text{population state that feeds} \\ \text{into state } n \text{ at time } t - \Delta t \end{array} \right) \end{aligned} \tag{2.3}$$

Notice how each event from the above list is multiplied by a connected (dependent) probabilistic state. These connected states have already been defined for us with Eq. 2.1 where we need only change the index and time argument to fix the description. We must then simply determine the probability of a source event occurring. Recall the source, S, should be thought of as "the probability of a source event occurring per unit time", and thus we may define the probability of a source event occurring in the time interval Δt as:

$$\left(\begin{array}{l} \text{Probability of 1 source} \\ \text{event occurring in } I_f \end{array} \right) = S\Delta t. \tag{2.4}$$

From Eq. 2.4 and keeping in mind that Δt is sufficiently small, we may utilize the conservation of probability to determine:

$$\left(\begin{array}{l} \text{Probability of no source} \\ \text{event occurring in } I_f \end{array} \right) = 1 - S\Delta t. \tag{2.5}$$

Now let us address the connected state probabilities of Eq. 2.3. The first one is the "probability of being in state n at time $t - \Delta t$", and by comparing that statement to Eq. 2.1, we find that that is equivalent to the quantity $P_n(t - \Delta t)$. The second connected state requires additional thought as to what the index (i.e., the connected state) actually is. Since every source event produces one and only one neutron, we require there to be $n - 1$ neutrons at time $t - \Delta t$ in order for there to be n neutrons at time t due to a source event occurring within I_f. Thus, the second connected probability statement, the "probability of being in a population state that feeds into state n at time $t - \Delta t$", equates to $P_{n-1}(t - \Delta t)$. Assembling these connected states with Eqs. 2.4 and 2.5, we may write down the probability balance for the radioactive decay process:

$$P_n(t) = (1 - S\Delta t)\, P_n(t - \Delta t) + S\Delta t P_{n-1}(t - \Delta t). \tag{2.6}$$

Given this probability balance, we may next rearrange by subtracting by $P_n(t-\Delta t)$ and dividing by Δt to find:

$$\frac{P_n(t)-P_n(t-\Delta t)}{\Delta t} = -SP_n(t-\Delta t) + SP_{n-1}(t-\Delta t). \tag{2.7}$$

If we next take the limit as $\Delta t \to 0$, the left-hand side of Eq. 2.7 is simply the limit definition of a derivative with respect to t. Thus, by performing said limit, we arrive at a linear first-order ordinary differential-difference equation satisfied by $P_n(t)$:

$$\frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = -SP_n(t) + SP_{n-1}(t), \qquad n = 0, 1, 2, \ldots, \infty. \tag{2.8}$$

Recall from the assumptions of Sec. 2.1, we assume there are no neutrons in the system at time $t = t_o$, this provides an initial condition:

$$P_n(t=t_o) = \delta_{n,0} = \begin{cases} 1 \text{ if } n = 0 \\ 0 \text{ if } n = 1, 2, 3, \ldots \end{cases} \tag{2.9}$$

where $\delta_{i,j}$ is the Kronecker delta function.

Equation 2.8 is categorized as the differential form of the Chapman-Kolmogorov equation or more commonly referred to as the Forward Master Equation (FME) for the radioactive decay process. This FME is downward coupled (i.e., is a function of the lower-state probability $P_{n-1}(t)$) and can therefore be solved for one probability at a time starting with $n = 0$ using the integrating factor method. As it turns out, this is a very special case of a more general class of FMEs which cannot be solved in such a straightforward manner. It is for this reason that we instead employ the Master equation algorithm outlined in Sec. 1.3 to initially witness the machinery of the algorithm in this simple setting. The next step in the solution process is to define and apply the probability generating function onto the FME, shown in the next section.

2.2.2 Equation for the Probability Generating Function

In this section, we employ a transformation method on the FME which effectively consolidates the infinite number of differential equations into a single equation for the transform function. The transform we use is called the probability generating function (PGF). The PGF is an attractive transform because it is essentially a power series representation of the PDF, which has a well-developed theory established for non-negative coefficients.

Proceeding, we define the PGF as

$$G(z,t) = \sum_{n=0}^{\infty} z^n P_n(t), \tag{2.10}$$

where z is the PGF transform variable and we restrict it to the domain: $\{z \in \mathbb{R} | 0 \leq z \leq 1\}$. Thus, by multiplying Eq. 2.8 by z^n and summing over all n, we have:

$$\sum_{n=0}^{\infty} z^n \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = -S\sum_{n=0}^{\infty} z^n P_n(t) + S\sum_{n=0}^{\infty} z^n P_{n-1}(t). \tag{2.11}$$

Next, we will work through each term followed by a transforming of the initial condition.

Starting with the left-hand side of Eq. 2.11, we may perform the following manipulations:

$$\begin{aligned}\sum_{n=0}^{\infty} z^n \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} &= \frac{\partial}{\partial t}\sum_{n=0}^{\infty} z^n P_n(t) \\ &= \frac{\partial G(z,t)}{\partial t},\end{aligned} \tag{2.12}$$

where going from the first to the second line in the above, we simply used the definition of the PGF and we use a partial derivative because we have an additional independent variable, z. This same comparison is made for the first term on the right-hand side and we need only consider the last term. Let us define the new index $m = n - 1$, which provides $n = m + 1$. When $n = 0$, $m = -1$ and when $n = \infty$, $m = \infty$. The last term may then be written as:

$$\begin{aligned}\sum_{n=0}^{\infty} z^n P_{n-1}(t) &= \sum_{m=-1}^{\infty} z^{m+1} P_m(t) \\ &= z\sum_{m=0}^{\infty} z^m P_m(t) \\ &= zG(z,t),\end{aligned} \tag{2.13}$$

where we note that $P_{m=-1}$ is not a real quantity (how can we have negative populations?) and we simply start the new sum at $m = 0$. Next, the initial condition is found by recalling the Kronecker delta, $\delta_{i,j}$, is 0 for all values of i except when $i = j$, which it then equals 1. Thus, we have:

$$\begin{aligned}\sum_{n=0}^{\infty} z^n P_n(t_o) &= \sum_{n=0}^{\infty} z^n \delta_{n,0} \\ &= z^0 \\ G(z,t_o) &= 1.\end{aligned} \tag{2.14}$$

Assembling the terms from Eqs. 2.12 and 2.13, we find a linear first-order partial differential equation (PDE) satisfied by the PGF:

$$\frac{\partial G(z,t)}{\partial t} = S(z-1)G(z,t) \tag{2.15}$$

with the initial condition

$$G(z,t_o) = 1. \tag{2.16}$$

We have gone from a system of ordinary differential-difference equations with an infinite number of equations, Eq. 2.8, to a single two-variable partial differential equation. The trade-off being that we no longer have to deal with an infinite set, but now we have to solve a PDE. In the next section, we demonstrate the solution method often employed when solving the PGF PDE.

2.2.3 Solution to the PGF PDE

We now task ourselves with solving the PGF PDE for the radioactive decay process given by Eq. 2.15. The PGF PDE is a linear PDE that is separable and can be solved using the Separation of Variables technique. As was mentioned near the end of Sec. 2.2.1, we choose to follow the methodology that will be employed for the more complicated equations we will see in later chapters of this primer. Instead of using separation of variables, we will solve Eq. 2.15 using the Method of

Characteristics (MoC) to show the reader how that method is employed and to give the reader an understanding of the Master equation solution algorithm in this simple setting.

Let us take the total derivative of $G(z(t),t)$ with respect to t:

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{\partial G}{\partial t} + \frac{\partial G}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t}. \tag{2.17}$$

If we now compare Eq. 2.17 with Eq. 2.15, we may infer two ordinary differential equations:

$$\frac{\mathrm{d}z}{\mathrm{d}t} = 0 \tag{2.18a}$$

$$\frac{\mathrm{d}G}{\mathrm{d}t} = S(z-1)G. \tag{2.18b}$$

Equation 2.18a informs us that z is a constant and not a function of t. Equation 2.18b is a separable ODE and can be solved by cross-multiplying and integrating to find:

$$\int_{G(z,t_o)}^{G(z,t)} \frac{\mathrm{d}G'}{G'} = S(z-1)\int_{t_o}^{t} \mathrm{d}t'. \tag{2.19}$$

Upon evaluating the integrals, we find

$$\ln\left(\frac{G(z,t)}{G(z,t_o)}\right) = S(z-1)(t-t_o). \tag{2.20}$$

Noting the initial condition and solving for $G(z,t)$ gives us a solution to the PGF PDE:

$$G(z,t) = \mathrm{e}^{S(z-1)(t-t_o)}. \tag{2.21}$$

The next step will be to find the number distribution using this solution, shown in the next section.

2.2.4 Inversion of the PGF

Now that we have a solution to the PGF PDE, Eq. 2.15, given by Eq. 2.47, we need to determine the neutron number distribution, $P_n(t)$. This can be done by recalling that, when we introduced G in Sec. 2.2.2, we referred to it as a power series representation of the PDF and thus we should be able to extract the PDF by expanding G into a power series.

The solution we have obtained for G is neatly contained in the exponential function, which has a well-known convergent power series given by:

$$\mathrm{e}^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}. \tag{2.22}$$

Let us then expand $G = \mathrm{e}^{-S(t-t_o)}\mathrm{e}^{S(t-t_o)z}$ in a Taylor series about $z = 0$ and write the first few terms:

$$\begin{aligned} G(z,t) &= \mathrm{e}^{-S(t-t_o)} \sum_{n=0}^{\infty} \frac{z^n \big(S(t-t_o)\big)^n}{n!} \\ &= \mathrm{e}^{-S(t-t_o)} \left[1 + zS(t-t_o) + z^2 \frac{\big(S(t-t_o)\big)^2}{2!} + z^3 \frac{\big(S(t-t_o)\big)^3}{3!} + \dots\right]. \end{aligned} \tag{2.23}$$

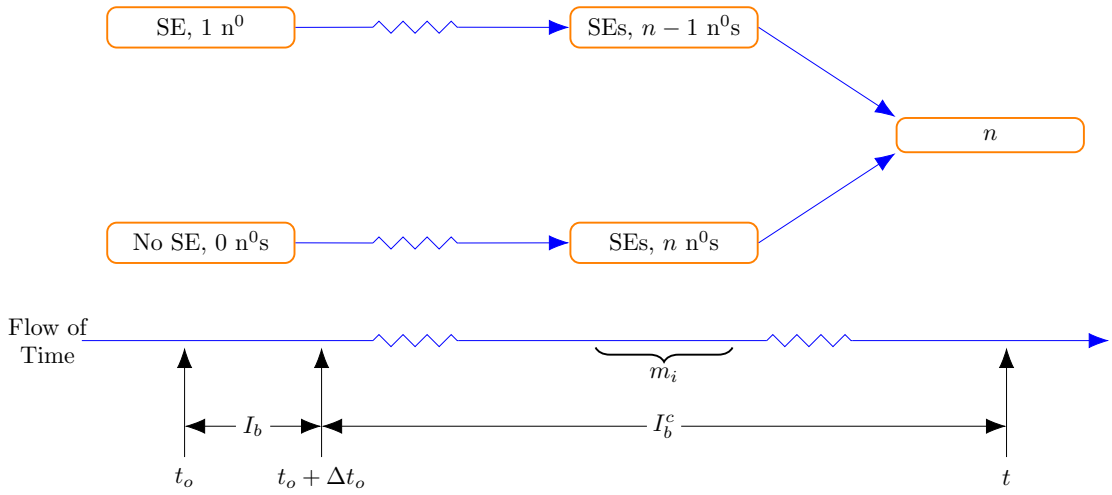


Figure 2.2: Mutually exclusive events that may occur in time interval I_b with their associated states, m_i, that must occur in time interval I_b^c for a singlet-emitting source in a neutron-transparent medium. SE = Source Event. Note the 'zig-zags' indicate an arbitrary passage of time. If a SE occurs in I_b, producing 1 n^0, then subsequent SEs occurring in I_b^c must produce $n-1$ n^{0}s. If no SE occurs in I_b, then subsequent SEs that occur in I_b^c must result in n n^{0}s.

By now comparing Eq. 2.23 with the original definition of G:

$$\begin{aligned} G(z,t) &= \sum_{n=0}^{\infty} z^n P_n(t) \\ &= P_0(t) + zP_1(t) + z^2P_2(t) + z^3P_3(t) + \ldots, \end{aligned} \tag{2.24}$$

we may determine the neutron number distribution by inspection:

$$P_n(t) = \frac{\big(S(t-t_o)\big)^n}{n!} \mathrm{e}^{-S(t-t_o)}, \tag{2.25}$$

which is the Poisson distribution with rate parameter $S(t-t_o)$. It is known that the radioactive decay process obeys Poisson statistics over a given time counting interval [41] and, as such this result is expected.

2.3 Backward Formulation

We now present the backward Master equation formulation for the radioactive decay model following the steps outlined in Sec. 1.3.

2.3.1 Probability Balance & Master Equation

The zeroth step of the backward approach requires defining the probability we wish to know:

$$\Theta_n(t|t_o) = \text{the probability of there existing } n \text{ neutrons within the system at time } t \text{ due to the introduction of a source of strength } S \text{ at an earlier time } t_o. \tag{2.26}$$

Historically, the Θ symbol is used to define the source-related probability in the BME while P is used when we consider single neutron fission chains without a source present. We will see in later chapters why the backward approach requires a different symbol for the single chain and source probabilities. We use notation used for conditional probabilities to define Θ_n, thus one could replace 'due to the' in Eq. 2.26 with 'conditioned on the'.

We define the time intervals of interest for the upcoming probability balance:

$$I_b = [t_o, t_o + \Delta t_o] \tag{2.27a}$$

$$I_b^c = [t_o + \Delta t_o, t] \tag{2.27b}$$

where we see that the entire time interval, from introduction of the source at t_o to observation of the system at t, is given by $I_b + I_b^c$. Also, we use the superscript c to denote the complement. With this, we must change our thinking a little bit from how we derived a probability balance in the forward approach. The first difference is that we are conducting a balance in the *first* collision interval, which is to say that we are starting from the very beginning as opposed to the forward approach which has the balance conducted at the very end of the total time interval. We will see that the approaches, though different, give the same answers. The list of mutually exclusive events that occur in the first collision interval, I_b, are the same as before:

1. No source event occurs
2. A source event occurs, producing 1 neutron.

Here is where we need to think different from the forward approach. The first collision interval, I_b, is quite small because Δt_o is very small while the difference in time between $t_o + \Delta t_o$ and t (i.e. I_b^c) is arbitrarily large. Thus, there could be additional source events that may occur in the remaining time I_b^c and we will need to include that possibility in our probability balance. To further illustrate this, Fig. 2.2 shows the events and how they may occur over the total time interval, where we note that the zig-zigs mean an arbitrary passage of time and SE stands for source event. In this figure, we see the list of events that may occur in I_b, followed by a passage of time in I_b^c where an arbitrary number of source events occurs and produces the necessary remaining neutrons needed to eventually arrive at n neutrons at t. These necessary number of neutrons are then the connected states to n, which are defined by the difference between n and the number of neutrons produced in I_b.

With this, we may define a probability balance in words:

$$\begin{aligned}\Theta_n(t|t_o) = &\begin{pmatrix}\text{Probability of no source}\\ \text{event occurring in } I_b\end{pmatrix} \times \begin{pmatrix}\text{Probability of subsequent source events}\\ \text{occurring in } I_b^c \text{ resulting in } n \text{ neutrons at } t\end{pmatrix} \\ &+ \begin{pmatrix}\text{Probability of 1 source event occurring}\\ \text{in } I_b \text{ resulting in 1 neutron at } t\end{pmatrix} \times \begin{pmatrix}\text{Probability of subsequent source events}\\ \text{occurring in } I_b^c \text{ resulting in } n-1 \text{ neutrons at } t\end{pmatrix}.\end{aligned} \tag{2.28}$$

Just as before, we can easily define the probability of a source event occurring in the short time Δt_o by recalling that the source, S, is defined as 'the probability of a source event occurring per unit

time', which results in the following:

$$\begin{pmatrix}\text{Probability of 1 source event occurring}\\ \text{in } I_b \text{ resulting in 1 neutron at } t\end{pmatrix} = S\Delta t_o \tag{2.29}$$

In truth, the time interval we multiply S by is $(t_o + \Delta t_o - t_o)$ as that is the width of I_b, but obviously the t_o's cancel. Next, we may define the complement of Eq. 2.29 using the conservation of probability to find:

$$\begin{pmatrix}\text{Probability of no source}\\ \text{event occurring in } I_b\end{pmatrix} = 1 - S\Delta t_o \tag{2.30}$$

Next, we need not consider explicit, singular events that may occur in I_b^c to write the subsequent probabilities. Let us first consider the 'probability of subsequent source events occurring in I_b^c resulting in n neutrons at t,' by changing the wording to the 'probability of there being n neutrons at time t due to the introduction of a source at time $t_o + \Delta t_o$.' We may make this equivalence because each source event is independent of all others. Similarly, let us alter the 'probability of subsequent source events occurring in I_b^c resulting in $n-1$ neutrons at t' to the 'probability of there being $n-1$ neutrons at time t due to the introduction of a source at time $t_o + \Delta t_o$.' Now by closely comparing the definition given by Eq. 2.26 with these re-wordings of the events that may occur in I_b^c, we find:

$$\begin{pmatrix}\text{Probability of subsequent source events}\\ \text{occurring in } I_b^c \text{ resulting in } n \text{ neutrons at } t\end{pmatrix} = \Theta_n(t|t_o + \Delta t_o) \tag{2.31a}$$

$$\begin{pmatrix}\text{Probability of subsequent source events}\\ \text{occurring in } I_b^c \text{ resulting in } n-1 \text{ neutrons at } t\end{pmatrix} = \Theta_{n-1}(t|t_o + \Delta t_o). \tag{2.31b}$$

Assembling these together, we obtain the first collision probability balance for a neutron source for a neutron-transparent medium:

$$\Theta_n(t|t_o) = (1 - S\Delta t_o)\Theta_n(t|t_o + \Delta t_o) + S\Delta t_o\Theta_{n-1}(t|t_o + \Delta t_o). \tag{2.32}$$

Next, we divide by Δt_o and subtract $\Theta_n(t|t_o + \Delta t_o)$ to find:

$$-\frac{\Theta_n(t|t_o + \Delta t_o) - \Theta_n(t|t_o)}{\Delta t_o} = -S\Theta_n(t|t_o + \Delta t_o) + S\Theta_{n-1}(t|t_o + \Delta t_o). \tag{2.33}$$

On the left-hand side, we have placed the $\Theta_n(t|t_o + \Delta t_o)$ in front of the $\Theta_n(t|t_o)$ to make the next step easier. If we now evaluate the limit as $\Delta t_o \to 0$, the LHS becomes the derivative of $\Theta_n(t|t_o)$ with respect to t_o, and we thus have:

$$-\frac{\partial\Theta_n(t|t_o)}{\partial t_o} = -S\Theta_n(t|t_o) + S\Theta_{n-1}(t|t_o), \tag{2.34}$$

which is the backward Master equation for the neutron number distribution in the presence of a radioactive source in a neutron-transparent medium. A striking difference between the BME and the FME given by Eq. 2.8 is the need to keep track of two time quantities: t_o and t. This is because t_o is the operational time variable (i.e., we are taking a derivative with respect to t_o, not t).

Finally, we need a terminal condition in order to solve this equation. Recall that we are assuming there are 0 neutrons in the system before the introduction of the source at t_o. Typically, we write

the 'final' condition as a limit to signify that we are 'bringing' the source introduction time up to the present time of observation, t. Thus, the final condition is:

$$\lim_{t_o \to t} \Theta_n(t|t_o) = \delta_{n,0} = \begin{cases} 1 \text{ if } n = 0 \\ 0 \text{ if } n = 1, 2, 3, \dots \end{cases} \tag{2.35}$$

where $\delta_{i,j}$ is the Kronecker delta function.

Equation 2.34 is the backward Master equation for the model under consideration. We note that the operational variable is the initial time and not the final time- a stark difference from the forward Master equation. The equation is an adjoint linear partial-differential-difference equation that is downward coupled and can therefore be solved. It is considered adjoint because the time derivative has a negative sign appended to it, and we will therefore need to integrate backwards in time (we will see this in action later)[3].

We note that, same as the forward approach, this equation may be solved by solving the $n = 0$ equation and moving on to $n = 1$, supplementing the Θ_0 solution, solving that equation and so on. We choose to present an alternative, seemingly more cumbersome, method in this setting to introduce the new-to-stochastic neutronics reader how we typically solve Master equations that are more complex than the one we just derived. In the next section, we transform the BME into a PDE for the probability generating function- an equation that is then solved via the Method of Characteristics.

2.3.2 Equation for the Probability Generating Function

The probability generating function (PGF) is defined as:

$$H(z, t|t_o) = \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o), \tag{2.36}$$

where again we use a different notation for the backward approach. The transform variable, z, is a real number with domain: $z \in [0, 1]$, which ensures absolute convergence.

We may transform the BME given by Eq. 2.34 by multiplying the equation by z^n and summing over all n to find:

$$-\sum_{n=0}^{\infty} z^n \frac{\partial \Theta_n(t|t_o)}{\partial t_o} = -S \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o) + S \sum_{n=0}^{\infty} z^n \Theta_{n-1}(t|t_o). \tag{2.37}$$

Note here that this effectively consolidates the infinite number of PDEs for Θ_n into a single equation. Let us now consider each term to write the above in terms of H. First, the derivative may be manipulated in the following manner:

$$\begin{aligned} \sum_{n=0}^{\infty} z^n \frac{\partial \Theta_n(t|t_o)}{\partial t_o} &= \frac{\partial}{\partial t_o} \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o) \\ &= \frac{\partial H(z, t|t_o)}{\partial t_o}. \end{aligned} \tag{2.38}$$

[3]For an in-depth discussion on the concept and applications of the adjoint in nuclear reactor theory, we recommend Lewins [38]

Next, the first term on the RHS is clearly $-SH$ and the second term requires a little more work. If we define a new index: $m = n - 1$, then $n = m + 1$ and the sum limits are $m = -1$ to $m = \infty$. The following manipulations may be performed:

$$\begin{aligned}\sum_{n=0}^{\infty} z^n \Theta_{n-1}(t|t_o) &= \sum_{m=-1}^{\infty} z^{m+1} \Theta_m(t|t_o) \\ &= z \sum_{m=0}^{\infty} z^m \Theta_m(t|t_o) \\ &= zH(z,t|t_o),\end{aligned} \tag{2.39}$$

where we note that $\Theta_{m=-1} = 0$ because a negative population number is non-physical. Finally, the final condition is transformed as follows:

$$\begin{aligned}\lim_{t_o \to t} \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o) &= \sum_{n=0}^{\infty} z^n \delta_{n,0} \\ &= z^0 \\ \lim_{t_o \to t} H(z,t|t_o) &= 1.\end{aligned} \tag{2.40}$$

Assembling the transformed quantities, we obtain a PDE for the PGF:

$$-\frac{\partial H(z,t|t_o)}{\partial t_o} = S(z-1)H(z,t|t_o) \tag{2.41}$$

with the final condition

$$\lim_{t_o \to t} H(z,t|t_o) = 1. \tag{2.42}$$

This equation is easily solved via separation of variables and then integration backwards in time. As we did for the forward case, we opt to show an alternative solution method via the Method of Characteristics. We do this because PGF equations in later chapters are solved via the MoC and not by the separation of variables method and thus it proves instructive for the reader still unfamiliar with the MoC.

2.3.3 Solution to the PGF PDE

The PGF PDE may be solved using the MoC. The basic idea is to write the PDE as a system of ODEs, which are then solved and a solution is assembled. To find the system of ODEs, let us consider the total derivative of H:

$$\frac{\mathrm{d}H}{\mathrm{d}t_o} = \frac{\partial H}{\partial t_o} + \frac{\partial H}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t_o}. \tag{2.43}$$

Comparing this equation to the BME given by Eq. 2.41, we may infer the system of ODEs as:

$$\frac{\mathrm{d}z}{\mathrm{d}t_o} = 0 \tag{2.44a}$$

$$\frac{\mathrm{d}H}{\mathrm{d}t_o} = S(z-1)H. \tag{2.44b}$$

These are often referred to as the characteristic equations. Equation 2.44a shows us that z is not a function of time and may therefore be treated as a constant with regard to the time integrals involved in solving Eq. 2.44b. On that note, Eq. 2.44b is a separable ODE that may be solved with the separation of variables method and integrating backwards in time to find:

$$-\int_{H(z,t|t)}^{H(z,t|t_o)} \frac{\mathrm{d}H'}{H'} = S(z-1)\int_t^{t_o} \mathrm{d}t'_o. \tag{2.45}$$

Evaluating the integrals yields

$$-\ln\left(\frac{H(z,t|t_o)}{H(z,t|t)}\right) = S(z-1)(t_o - t). \tag{2.46}$$

Then by solving for $H(z,t|t_o)$, we find the desired solution to the BME:

$$H(z,t|t_o) = \mathrm{e}^{S(z-1)(t-t_o)}. \tag{2.47}$$

The next step will be to find the number distribution using this solution, shown in the next section. Note the resemblance between this solution and that of the forward approach given by Eq. 2.47 ($G(z,t) = \mathrm{e}^{S(z-1)(t-t_o)}$). This comes as no surprise since both the backward and forward approaches give the same solutions, the only difference being the time variable that is used.

2.3.4 Inversion of the PGF

As we did in the forward approach, we need to invert the expression for $H(z,t|t_o)$ to extract the number distribution $\Theta_n(t|t_o)$. This can be done by expanding H in a Taylor series about $z = 0$. Note that z appears in the exponential function and we therefore need to expand this function, which has the Taylor series:

$$\mathrm{e}^x = \sum_{k=0}^{\infty} \frac{x^k}{k!}. \tag{2.48}$$

Then by slightly rewriting H, we then expand $H = \mathrm{e}^{-S(t-t_o)}\mathrm{e}^{S(t-t_o)z}$ in a Taylor series about $z = 0$ whose first few terms are:

$$\begin{aligned} H(z,t|t_o) &= \mathrm{e}^{-S(t-t_o)} \sum_{n=0}^{\infty} \frac{z^n (S(t-t_o))^n}{n!} \\ &= \mathrm{e}^{-S(t-t_o)} \left[1 + zS(t-t_o) + z^2 \frac{(S(t-t_o))^2}{2!} + z^3 \frac{(S(t-t_o))^3}{3!} + \ldots\right]. \end{aligned} \tag{2.49}$$

By now comparing Eq. 2.49 with the original definition of H:

$$\begin{aligned} H(z,t|t_o) &= \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o) \\ &= \Theta_0(t|t_o) + z\Theta_1(t|t_o) + z^2\Theta_2(t|t_o) + z^3\Theta_3(t|t_o) + \ldots, \end{aligned} \tag{2.50}$$

we may determine the neutron number distribution by inspection:

$$\Theta_n(t|t_o) = \frac{(S(t-t_o))^n}{n!}\mathrm{e}^{-S(t-t_o)}. \tag{2.51}$$

This gives the expected solution as a Poisson distribution (for reasons explained in Sec. 2.2.4), which is no different from the solution obtained in the forward approach.

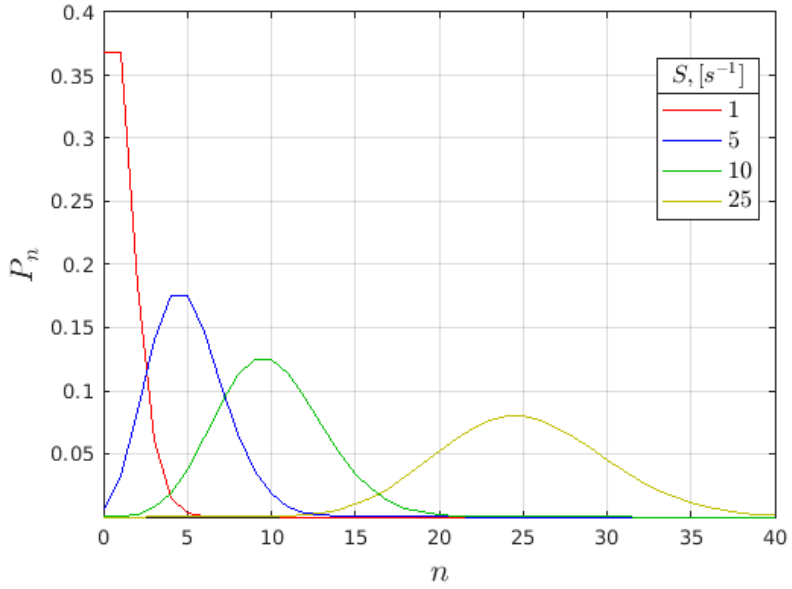


Figure 2.3: Poisson distributions for varying source strengths.

2.4 Example & Discussion

We now consider an example system with a source and no neutron interactions. Figure 2.3 shows Eq. 2.25 (or 2.51) plotted for $t = 1\ s$, $t_o = 0\ s$, and several different source strengths. Thus, because the time difference is the same for each case ($t - t_o = 1\ s$), this figure demonstrates the effects of source strength on the total number of source events that have occurred up to that point in time (or total number of neutrons in the system). For the weakest source of $S = 1s^{-1}$, the probability of there being no source events up to that time is the greatest than the others. This is consistent with the definition of S being the probability per unit time that a source event occurs and therefore the lesser the magnitude, the less likely an event will occur. As the source strength is increased, the bulk of the distribution increases as well, as expected. We will see this behavior for all number distributions with a source present. On a final note, we could also keep the source strength constant (i.e., set it equal to $S = S_o$ for all the cases) and then change the time $t - t_o$ to 1, 5, 10, and 25 seconds and the plot will look identical to Fig. 2.3. This would tell us that, for a given source strength, as time progresses the total number of source events that occur up to that point will always be increasing and will be Poisson distributed.

Chapter 3

Binary Fission Model, No Capture, with a Source

In this chapter, we build upon the concepts we introduced in the previous chapter by considering certain neutron effects within the model. Section 3.1 covers the aspects of the model we are now considering. Section 3.2 demonstrates the MESA for the Forward Formulation while Sec. 3.3 shows how to apply the MESA for the Backward Formulation. As we will see, the algorithm is essentially identical to the last chapter, but will become more mathematically involved due to the additional physics we account for.

3.1 The Model

The system is the same as before, but we now allow neutrons to collide with the nuclei of the system and, upon colliding, induce fission events. We summarize the model below:

- instantly after a fission event occurs, we allow for exactly two neutrons to emerge and we call this the Binary Fission Model (BFM),
- neutrons emitted from induced fission travel with speed v,
- we still ignore other neutron collision events such as scattering,
- the system has a neutron source of strength S, which emits one neutron per source event, traveling at speed v.

3.2 Forward Formulation

3.2.1 Probability Balance & Master Equation

We begin by defining the probabilistic quantity we wish to obtain:

$$P_n(t) = \text{the probability of there existing } n \text{ neutrons within the system at time } t \tag{3.1}$$

where we note the definition is now a little more ambiguous compared to Eq. 2.1. We do this now because there are essentially two possible initial conditions that could cause there to be n neutrons

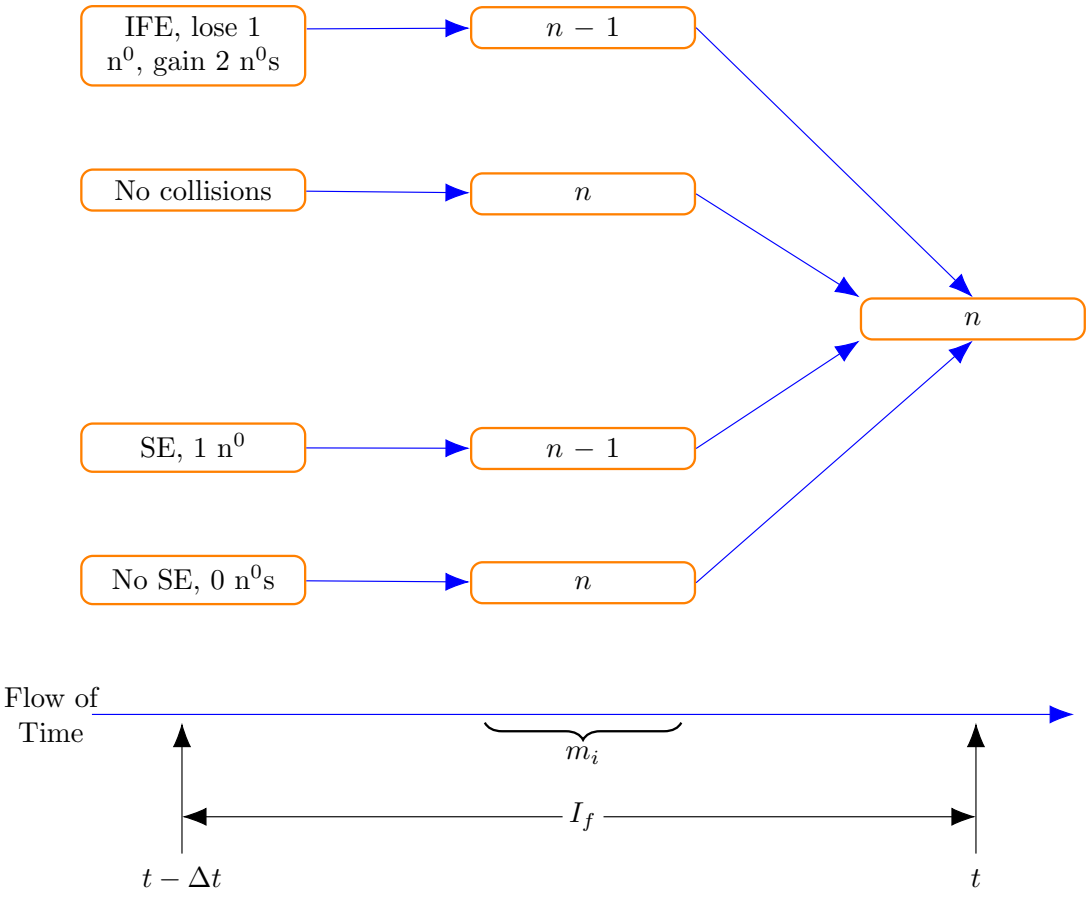


Figure 3.1: Forward formulation event tree for the BFM with a source and without capture. Note IFE = induced fission event and SE = source event.

in the system at time t. First, there could be no discernible source within the system, but there are m neutrons which could give rise to n neutrons at time t. Second, there could be a source and we would therefore assume $m = 0$ from the first example.

To determine $P_n(t)$, we use knowledge of the possible states the system could be occupying a short time before t given by $t-\Delta t$. Thus we will conduct a probability balance over the time domain:

$$I_f = [t - \Delta t, t], \tag{3.2}$$

where the subscript f refers to this being the forward time interval. We assume Δt is sufficiently small enough that only a single source event or neutron collision may reasonably occur within it. In constructing the probability balance, let us first state the possible events that may occur within the short time interval I_f:

1. A neutron collides and is absorbed, causes an induced fission event (IFE), and two neutrons are emitted

2. A source event occurs, producing 1 neutron

3. No event occurs (no neutrons collide with nuclei and no source events occur)

The event tree in Fig. 3.1 shows this list in action. In the figure, we see the event that may occur in the far-left bubbles with the resultant number of neutrons that emerge, followed by the intermediary state m_i- the i^{th} state that is event-connected to state n- which we use to aid in the forthcoming probability balance. Note that this event tree has grown and we see that Fig. 2.1 is now but a subset of this tree. Using the list above, we may write the probability balance in words as follows:

$$\begin{aligned} P_n(t) = &\left(\begin{array}{c} \text{Probability of no source} \\ \text{event occurring in } I_f \end{array} \right) \times \left(\begin{array}{c} \text{Probability that none of} \\ \text{the } n \text{ n}^0\text{s collide in } I_f \end{array} \right) \times \left(\begin{array}{c} \text{Probability of being in} \\ \text{state } n \text{ at time } t - \Delta t \end{array} \right) \\ &+ \left(\begin{array}{c} \text{Probability of 1 source} \\ \text{event occurring in } I_f \end{array} \right) \times \left(\begin{array}{c} \text{Probability of being in a} \\ \text{population state that feeds} \\ \text{into state } n \text{ at time } t - \Delta t \end{array} \right) \\ &+ \left(\begin{array}{c} \text{Probability of } n-1 \text{ n}^0\text{s} \\ \text{colliding in } I_f, \text{ causing} \\ \text{an IFE} \end{array} \right) \times \left(\begin{array}{c} \text{Probability of being in} \\ \text{population state } n-1 \\ \text{at time } t - \Delta t \end{array} \right) \end{aligned} \tag{3.3}$$

Notice how each event from the above list is multiplied by a connected (dependent) probabilistic state. These connected states have already been defined for us with Eq. 3.1 where we need only change the index and time argument to fix the description. We must next determine the probability of a source event occurring, the probability of no neutrons colliding, and the probability of one neutron colliding and inducing a fission. As before, the source, S, should be thought of as "the probability of a source event occurring per unit time", and thus we may define the probability of a source event occurring in the time interval Δt as:

$$\left(\begin{array}{c} \text{Probability of 1 source} \\ \text{event occurring in } I_f \end{array} \right) = S\Delta t. \tag{3.4}$$

From Eq. 3.4 and keeping in mind that Δt is sufficiently small, we may utilize the conservation of probability to determine:

$$\left(\begin{array}{c} \text{Probability of no source} \\ \text{event occurring in } I_f \end{array} \right) = 1 - S\Delta t. \tag{3.5}$$

Next, we need to determine the probability that a neutron collides and induces a fission. Recall that the reaction rate of interaction x, λ_x, can be thought of as the "probability that event type x occurs per unit time per neutron". Thus, for a single neutron propagating in the time interval Δt, we have:

$$\left(\begin{array}{c} \text{Probability that 1} \\ \text{n}^0 \text{ collides in } I_f \end{array} \right) = \lambda_f \Delta t. \tag{3.6}$$

Similar to how we arrived at Eq. 3.5, we use the conservation of probability to determine the probability that one neutron does not collide in I_f as: $1 - \lambda_f \Delta t$. Notice that that expression is for a *single* neutron, and we therefore need to multiply $1 - \lambda_f \Delta t$ to itself for each neutron present in the system. If no collisions have occurred in Δt, then there must already be n neutrons in the system at $t - \Delta t$. From this, we find:

$$\left(\begin{array}{c} \text{Probability that none of} \\ \text{the } n \text{ n}^0\text{s collide in } I_f \end{array} \right) = (1 - \lambda_f \Delta t)^n . \tag{3.7}$$

Note that λ_f in the above will become $(\lambda_f + \lambda_c + \ldots)$ as we include more interactions in later chapters. Following that same multiplicative process, if we want to know the probability that $n-1$ neutrons induce a fission in Δt, we need to multiply $\lambda_f \Delta t$ by itself $n-1$ times to find:

$$\left(\begin{array}{c} \text{Probability of } n-1 \text{ n}^0\text{s} \\ \text{colliding in } I_f\text{, causing} \\ \text{an IFE} \end{array} \right) = (n-1)\lambda_f \Delta t. \tag{3.8}$$

Now let us address the connected state probabilities of Eq. 2.3. The first one is the "probability of being in state n at time $t - \Delta t$", and by comparing that statement to Eq. 2.1, we find that that is equivalent to the quantity $P_n(t - \Delta t)$. The second connected state requires additional thought as to what the index (i.e., the connected state) actually is. Since every source event produces one and only one neutron, we require there to be $n-1$ neutrons at time $t - \Delta t$ in order for there to be n neutrons at time t due to a source event occurring within I_f. Thus, the second connected probability statement, the "probability of being in a population state that feeds into state n at time $t - \Delta t$", equates to $P_{n-1}(t - \Delta t)$. The final connected state requires $n + 1 - 2$ neutrons- $+1$ because we lose the inducing neutron when it is absorbed and the -2 because we end up with 2 neutrons released from the fission event.

Assembling these connected states with Eqs. 3.4 through 3.7, we may write down the probability balance for this model:

$$P_n(t) = (1 - S\Delta t)\left(1 - \lambda_f \Delta t\right)^n P_n(t - \Delta t) + S\Delta t P_{n-1}(t - \Delta t) + (n-1)\lambda_f \Delta t P_{n-1}(t - \Delta t). \tag{3.9}$$

Before continuing, we may simplify the "no event" probability by expanding $(1 - \lambda_f \Delta t)^n$ in a Taylor series about $\lambda_f \Delta t = 0$ for sufficiently small Δt:

$$\begin{aligned} (1 - \lambda_f \Delta t)^n =& 1 - n\lambda_f \Delta t + \frac{1}{2} n(n-1)\left(\lambda_f \Delta t\right)^2 - \frac{1}{6} n(n-1)(n-2)\left(\lambda_f \Delta t\right)^3 + \cdots \\ =& 1 - n\lambda_f \Delta t + \mathcal{O}\left(\left[\Delta t\right]^2\right), \end{aligned} \tag{3.10}$$

where $\mathcal{O}$ is the Big-O notation for the truncated Taylor series' limiting behavior. We may then write:

$$(1 - S\Delta t)\left(1 - \lambda_f \Delta t\right)^n = 1 - \left(S + n\lambda_f\right)\Delta t + \mathcal{O}\left(\left[\Delta t\right]^2\right). \tag{3.11}$$

With the probability balance, Eq. 3.9, we may rearrange by subtracting by $P_n(t - \Delta t)$ and dividing by Δt to find:

$$\frac{P_n(t) - P_n(t - \Delta t)}{\Delta t} = -\big(S + n\lambda_f - \mathcal{O}\left(\Delta t\right)\big)P_n(t - \Delta t) + \big(S + (n-1)\lambda_f\big)P_{n-1}(t - \Delta t). \tag{3.12}$$

If we next take the limit as $\Delta t \to 0$, the left-hand side of Eq. 2.7 is simply the limit definition of a derivative with respect to t. We then arrive at a linear first-order ordinary differential-difference equation satisfied by $P_n(t)$:

$$\frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = -\big(S + n\lambda_f\big)P_n(t) + \big(S + (n-1)\lambda_f\big)P_{n-1}(t), \tag{3.13}$$

with $n = 0, 1, 2, \ldots$. Recall from the assumptions of Sec. 3.1, we allow for an arbitrary number of neutrons, m, in the system at time $t = t_o$, this provides an initial condition:

$$P_n(t = t_o) = \delta_{n,m} = \begin{cases} 1 \text{ if } n = m \\ 0 \text{ if } n \neq m \end{cases} \tag{3.14}$$

where $\delta_{i,j}$ is the Kronecker delta function. Equation 2.8 is the Forward Master Equation (FME) for the model defined in Sec. 3.1.

3.2.2 Equation for the Probability Generating Function

We now transform the infinite set of differential-difference equations given by Eq. 3.13 into a single PDE satisfied by the probability generating function (PGF), defined as:

$$G(z,t) = \sum_{n=0}^{\infty} z^n P_n(t). \tag{3.15}$$

We will also make use of the z-derivative of G, which is written as:

$$\frac{\partial G(z,t)}{\partial z} = \sum_{n=0}^{\infty} n z^{n-1} P_n(t). \tag{3.16}$$

The transformation is facilitated by multiplying Eq. 3.13 by z^n and summing over all n to find:

$$\sum_{n=0}^{\infty} z^n \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = -\sum_{n=0}^{\infty} z^n \big(S + n\lambda_f\big) P_n(t) + \sum_{n=0}^{\infty} z^n \big(S + (n-1)\lambda_f\big) P_{n-1}(t). \tag{3.17}$$

As before, the LHS is simply $\partial G / \partial t$ and the first term on the RHS is $-SG$. The next term on the RHS is converted as follows:

$$\begin{aligned} \lambda_f \sum_{n=0}^{\infty} n z^n P_n(t) &= \frac{z}{z} \lambda_f \sum_{n=0}^{\infty} n z^n P_n(t) \\ &= z\lambda_f \sum_{n=0}^{\infty} n z^{n-1} P_n(t) \\ &= z\lambda_f \frac{\partial G(z,t)}{\partial z}, \end{aligned} \tag{3.18}$$

where we simply multiplied by z/z in order to make it more clear that this term is related to the partial derivative of G with respect to z as given by Eq. 3.16. This trick should be kept in mind when a coefficient of n shows up in the sum. For the next term, we use an index shift: $m = n - 1$:

$$\begin{aligned} S \sum_{n=0}^{\infty} z^n P_{n-1}(t) &= S \sum_{m=0}^{\infty} z^{m+1} P_m(t) \\ &= zS \sum_{m=0}^{\infty} z^m P_m(t) \\ &= zSG(z,t), \end{aligned} \tag{3.19}$$

where we note that when $n = 0$ and thus $m = -1$ gives an unrealistic probability P_{-1}, and we therefore set $m = 0$ as the lower sum limit. The final term requires an index shift as well. Define $m = n - 1$, to find:

$$\begin{aligned} \lambda_f \sum_{n=0}^{\infty} (n-1) z^n P_{n-1}(t) &= z\lambda_f \sum_{m=0}^{\infty} m z^m P_m(t) \\ &= \frac{z}{z} z\lambda_f \sum_{m=0}^{\infty} m z^m P_m(t) \\ &= z^2 \lambda_f \frac{\partial G(z,t)}{\partial z}, \end{aligned} \tag{3.20}$$

where we multiplied by z/z to get the sum into terms of the derivative of G with respect to z.

Assembling Eqs. 3.18 through 3.20 yields the PGF PDE:

$$\frac{\partial G(z,t)}{\partial t} = \lambda_f \left(z^2 - z\right) \frac{\partial G(z,t)}{\partial z} + S(z-1)G(z,t) \tag{3.21}$$

with initial condition given by:

$$G(z,t_o) = z^m, \tag{3.22}$$

where m is the initial neutron population in the system.

Notice now that Eq. 3.21 is equivalent to the previous PGF PDE, Eq. 2.15, but now with the $\lambda_f(z^2 - z)\,\partial G/\,\partial z$ term included. This new term has a λ_f associated with it and should therefore be thought of as the neutron interaction effects that are now included in this model. As we add more neutron interactions in later chapters, we will see the coefficient of $\partial G/\,\partial z$ evolve into a more complicated expression to account for additional physics. On that note, the $S(z-1)G$ term appears the same as before because there are no changes to the nature/character of the source. Once we allow for the source to emit more than one particle per event, we will see this term change as well. Just as before, we solve this first-order linear hyperbolic PDE using the Method of Characteristics, shown in the next section.

3.2.3 Solution to PGF PDE

To arrive at a solution to the PGF PDE given by Eq. 3.21, we use the Method of Characteristics. By taking the total derivative of G with respect to t,

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{\partial G}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t} + \frac{\partial G}{\partial t} \tag{3.23}$$

and comparing with the PGF PDE, we may write down the characteristic equations:

$$\frac{\mathrm{d}z}{\mathrm{d}t} = -\lambda_f \left(z^2 - z\right) \tag{3.24a}$$

$$\frac{\mathrm{d}G}{\mathrm{d}t} = S(z-1)G. \tag{3.24b}$$

Note now that z is not a constant like it was when no neutron interactions were allowed. Equation 3.24a is a Bernoulli ODE of order 2 and is solvable. For a k-order Bernoulli ODE, we make the substitution $y = z^{1-k}$, which has the derivative:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = (1-k)z^{-k}\frac{\mathrm{d}z}{\mathrm{d}t}. \tag{3.25}$$

Plugging these into Eq. 3.24a gives a linear inhomogeneous first-order ODE:

$$\frac{1}{1-k}\frac{\mathrm{d}y}{\mathrm{d}t} - \lambda_f y = \lambda_f. \tag{3.26}$$

Using $k = 2$, the integrating factor technique provides y, from which we may obtain z to find:

$$z(t) = \frac{z_o}{z_o + (1-z_o)\exp\left\{-\lambda_f(t-t_o)\right\}}, \tag{3.27}$$

where we have defined $z_o = z(t_o)$ as the initial value of $z(t)$.

Next, Eq. 3.24b is separable and can be integrated directly to find the expression

$$G(z,t) = G(z_o,t_o)\exp\left\{S\int_{t_o}^{t}\mathrm{d}t'\,(z(t')-1)\right\}. \tag{3.28}$$

Thus, by inserting Eq. 3.27 into the integral above, we can find a solution for G which we will then be able to use to find $P_n(t)$.

It is at this point that we consider two separate cases for which the initial condition changes:

1. The case where there is no source (by setting $S = 0$) and there is a single initial neutron in the system (set $m = 1$ in Eq. 3.22).
2. The case with a source present but no initial neutrons within the system (set $m = 0$ in Eq. 3.22).

These two cases are of importance because, well, they are fundamental. To elaborate, we consider case 1 to better understand the effects a single neutron and its progeny will have on the system. One clear concern is understanding the probability that a single neutron could initiate a fission chain that makes a reactor go supercritical- putting lives and the environment at risk. Case 2 is useful for modeling a system with, say, a spontaneous fission source and we may wish to know how much moderator/shield/absorber we may need in an experimental set-up. Further, the single chain case is a sub-set of the source case in that every source event initiates individual neutron chains, each of which may be modeled by the results of Case 1. With that, let us consider each case separately below.

Single Chain Solution

By setting $m = 1$ in Eq. 3.22 and setting $S = 0$ in Eq. 3.28, we find the expression for G:

$$G(z,t) = G(z_o,t_o) = z_o. \tag{3.29}$$

This tells us that the solution G is a constant along the characteristic curve and is defined by the initial condition z_o. We could have also arrived at this expression by inspecting the $S = 0$ case of Eq. 3.24b: $\mathrm{d}G/\,\mathrm{d}t = 0$, which tells us that the solution is a constant.

Proceeding, we now need an expression for z_o, which is obtained using Eq. 3.27 to find:

$$z_o = \frac{z\mathrm{e}^{-\lambda_f(t-t_o)}}{1+z\left(\mathrm{e}^{-\lambda_f(t-t_o)}-1\right)}. \tag{3.30}$$

Thus, we find the solution:

$$G(z,t) = \frac{z\mathrm{e}^{-\lambda_f(t-t_o)}}{1-z\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)}. \tag{3.31}$$

Singlet-Emitting Source Solution

For the source case, we simply set $m = 0$ in the initial condition, Eq. 3.22. This simplifies our solution expression to:

$$G(z,t) = \exp\left\{S\int_{t_o}^{t}\mathrm{d}t'\,(z(t')-1)\right\}. \tag{3.32}$$

The integral in the above may be computed with the aid of Eq. 3.27 to find:

$$\begin{aligned} S\int_{t_o}^{t} \mathrm{d}t' \left(z(t')-1\right) &= S\int_{t_o}^{t} \mathrm{d}t' \left(-1+\frac{z_o}{z_o+(1-z_o)\mathrm{e}^{-\lambda_f(t'-t_o)}}\right) \\ &= -S(t-t_o)+\frac{S}{\lambda_f}\ln\left[1+z_o\left(\mathrm{e}^{+\lambda_f(t-t_o)}-1\right)\right]. \end{aligned} \tag{3.33}$$

Next, we eliminate z_o from the above using Eq. 3.30 to find, after some algebra:

$$G(z,t) = \mathrm{e}^{-S(t-t_o)}\left[1-z\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)\right]^{-S/\lambda_f}. \tag{3.34}$$

3.2.4 Inversion of the PGF

As was done in the previous chapter, Sec. 2.2.4, we invert G to obtain P_n by Taylor expanding the expressions, Eqs. 3.31 and 3.34, about $z = 0$.

Single Chain Solution

We aim to invert Eq. 3.31, which can be done by rearranging and Taylor expanding about $z = 0$:

$$\begin{aligned} G(z,t) &= z\mathrm{e}^{-\lambda_f(t-t_o)}\left[1-z\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)\right]^{-1} \\ &= z\mathrm{e}^{-\lambda_f(t-t_o)}\sum_{n=0}^{\infty}\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)^n z^n \end{aligned} \tag{3.35}$$

where we note that this expansion is convergent because the quantity $(1-\mathrm{e}^{-\lambda_f(t-t_o)})$ is always bounded between 0 and 1 and therefore the entire bracketed quantity on the first line of Eq. 3.35 is also bounded between 0 and 1 for all t and all $z \in [0,1]$. Let us absorb the z in the front of the expression of Eq. 3.35 into the sum, define the index $m = n+1$ to find (and rename the index $m \to n$):

$$G(z,t) = \mathrm{e}^{-\lambda_f(t-t_o)}\sum_{n=1}^{\infty}\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)^{n-1} z^n \tag{3.36}$$

By now comparing Eq. 3.36 with the original definition of the PGF: $G(z,t) = \sum_{n=0}^{\infty} z^n P_n(t)$, we may extract the neutron number PDF for a single chain to find:

$$P_n(t) = \mathrm{e}^{-\lambda_f(t-t_o)}\left[1-\mathrm{e}^{-\lambda_f(t-t_o)}\right]^{n-1} \tag{3.37}$$

for $n = 1, 2, 3, \ldots$. Note that the value for $n = 0$ is $P_0(t) = 0$ because we have a single initial neutron that can only induce fissions, thus the chain will not die away because we have not allowed for any mechanism to do so. We may also verify the initial condition by setting $t = t_o$ to find $P_n(t_o) = \delta_{n,1} = 0^{n-1}$. Thus, 0^{n-1} is equal to 0 except when $n = 1$, whence $0^0 = 1$, proving the initial condition is satisfied.

Singlet-Emitting Source Solution

The source case is obtained by first defining

$$\eta = \frac{S}{\lambda_f} \tag{3.38}$$

for brevity. This parameter is referred to Bell's parameter in honor of G. I. Bell. We will be seeing more developed versions of this parameter in later chapters. Equation 3.34 may be Taylor expanded about $z = 0$ to yield:

$$\begin{aligned} G(z,t) &= \mathrm{e}^{-S(t-t_o)} \left[1 - z\left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)\right]^{-\eta} \\ &= \mathrm{e}^{-S(t-t_o)} \sum_{n=0}^{\infty} \frac{\eta(\eta+1)\cdots(\eta+n-1)}{n!} \left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)^n z^n. \end{aligned} \tag{3.39}$$

This series is convergent for the same reasons described in the single chain inversion section above. Once again, if we compare the above expression with the original definition of the PGF: $G(z,t) = \sum_{n=0}^{\infty} z^n P_n(t)$, we find the neutron number distribution in the presence of a singlet-emitting source. Noting the identity:

$$\eta(\eta+1)\cdots(\eta+n-1) = \frac{\Gamma(\eta+n)}{\Gamma(\eta)}, \tag{3.40}$$

where $\Gamma(\cdot)$ is the gamma function[1], the number distribution is stated as:

$$P_n(t) = \mathrm{e}^{-S(t-t_o)} \frac{\Gamma(\eta+n)}{n!\Gamma(\eta)} \left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)^n. \tag{3.41}$$

We may verify the initial condition, $P_n(t_o) = \delta_{n,0}$, by setting $t = t_o$ to find $P_n(t_o) = \Gamma(\eta + n)/(n!\Gamma(\eta))0^n$. Thus, 0^n is only non-zero when $n = 0$, whence $0^0 = 1$- verifying the initial condition.

3.3 Backward Formulation

We now present the backward Master equation formulation for this model following the steps outlined in Sec. 1.3. Aside from the additional physics, we now run into the first major difference in how to correctly conduct the backward formulation and how we solve this problem. We must first write down the probability balance for a single neutron without any sources present (this is equivalent to the single neutron initial condition problem for the forward formulation, but the probability balance is conducted in the first collision interval). We then write down a separate probability balance for the case of a source without any initial neutrons present. As we will see, the source problem will be a function of the single chain problem's solution. This is because a source is producing single chains with every source event, whence those chains go on to propagate independently from one another.

The reason we must write down two separate balance equations has to do with the way we pose the question, "How does the system behave probabilistically?" Well, if we have a source present, we will see that we need to single chain solution to correctly answer that question. If we instead start with writing the single chain case with a source, like we do in the forward formulation, we will find an equation that describes the probabilistic behavior of the population for which a single

[1]The gamma function has a rich history dating back to D. Bernoulli, C. Goldbach, and L. Euler of the 1720's. In essence, it is the generalization of the factorial function to non-integer numbers and complex numbers [44].

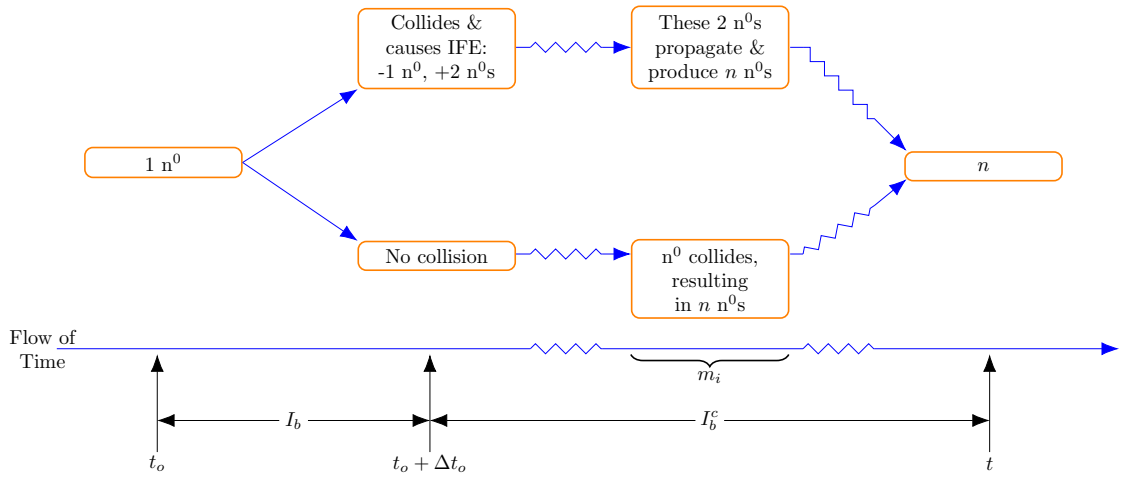


Figure 3.2: Mutually exclusive events that may occur in time interval I_b with their associated states, m_i, that must occur in time interval I_b^c for a single initiating neutron. IFE = Induced Fission Event. Note the 'zig-zags' indicate an arbitrary passage of time. If the initial n^0 collides in I_b, causing an IFE and producing 2 n^{0}s, then those 2 n^{0}s must propagate through I_b^c must result in n n^{0}s. If no collision occurs in I_b, then the initial n^0 must propagate in I_b^c, ultimately resulting in n n^{0}s.

source event occurs at exactly the initial time (i.e., the initial neutron is treated as a source event with a known time) along with the single event probability that occurs in I_b and the other arbitrary source events that occur randomly throughout I_b^c. Clearly, this scenario has no direct reference to a real *measurable* situation, where we would need to know the exact moment a single event occurs which is far too restrictive. From a mathematical point of view, the solution to such a probability balance would be non-unique because it would be an underdetermined equation (one equation with two unknowns).

We proceed by conducting the probability balances for the two cases: the single chain case and the source case. We then continue the MESA for both cases, solving the single chain equation first since the source case is a function of the single chain solution.

3.3.1 Probability Balance & Master Equation

As before, we define the time intervals of interest for the upcoming probability balances:

$$I_b = [t_o, t_o + \Delta t_o] \tag{3.42a}$$

$$I_b^c = [t_o + \Delta t_o, t] \tag{3.42b}$$

where we see that the entire time interval, from introduction of the source at t_o to observation of the system at t, is given by $I_b + I_b^c$. Also, we use the superscript c to denote the complement.

Single Chain

We begin by defining the probability we wish to know:

$$P_n(t|t_o) = \text{the probability of there existing } n \text{ neutrons within the system at time } t \text{ due to the introduction of a single neutron at an earlier time } t_o. \tag{3.43}$$

Recall that we are conducting a balance in the *first* collision interval (i.e., within the time interval defined by I_b). For the single initial neutron, the list of mutually exclusive events that occur in the first collision interval, I_b, are:

1. the neutron does not collide with a nucleus composing the medium,
2. the neutron does collide, inducing a fission event and producing 2 neutrons.

Let us again proceed with a cautionary note. We assume Δt_o is sufficiently small such that if a collision occurs the resulting neutrons will not interact with the system. Also, although Δt_o is very small, the difference in time between $t_o + \Delta t_o$ and t (i.e. I_b^c) is arbitrarily large. Thus, there could be additional events that may occur in the remaining time I_b^c and we will need to include that possibility in our probability balance. To further illustrate this, Fig. 3.2 shows the events and how they may occur over the total time interval, where we note that the zig-zigs mean an arbitrary passage of time and IFE stands for induced fission event. In this figure, we see the list of events that may occur in I_b, followed by a passage of time in I_b^c where the neutron chain propagates ultimately resulting in n neutrons at t. For the case of an IFE occurring in I_b, those 2 neutrons will propagate and each branch will produce a population n_1 and n_2 such that $n_1 + n_2 = n$ in order for that probability set to contribute to $P_n(t|t_o)$.

The probability balance in words is then:

$$\begin{aligned} P_n(t|t_o) = &\begin{pmatrix}\text{Probability the initial n}^0\\ \text{does not collide in } I_b\end{pmatrix} \times \begin{pmatrix}\text{Probability the initial n}^0 \text{ collides}\\ \text{in } I_b^c, \text{ resulting in } n \text{ neutrons at } t\end{pmatrix} \\ &+ \begin{pmatrix}\text{Probability initial n}^0 \text{ collides in } I_b,\\ \text{causing an IFE, producing 2 n}^0\text{s}\end{pmatrix} \times \begin{pmatrix}\text{Probability those 2 n}^0\text{s produce } n_1 \text{ and}\\ n_2 \text{ n}^0\text{s, such that } n_1 + n_2 = n, \text{ in } I_b^c\end{pmatrix}. \end{aligned} \tag{3.44}$$

We can define the probability of a collision occurring in I_b by noting that the only event that will occur following a collision is an IFE, thus we find:

$$\begin{pmatrix}\text{Probability initial n}^0 \text{ collides}\\ \text{in } I_b \text{ causing an IFE}\end{pmatrix} = \lambda_f \Delta t_o \tag{3.45}$$

It follows then that the probability of not colliding in I_b is:

$$\begin{pmatrix}\text{Probability initial n}^0\\ \text{does not collide in } I_b\end{pmatrix} = 1 - \lambda_f \Delta t_o \tag{3.46}$$

Next, we need not consider explicit, singular events that may occur in I_b^c to write the subsequent probabilities. Let us first consider the 'probability the initial neutron collides in I_b^c, resulting in n neutrons' by changing the wording to the 'probability of there being n neutrons at time t due to the introduction of a neutron at time $t_o + \Delta t_o$.' Similarly, let us alter the 'probability those 2 neutrons produce n_1 and n_2 neutrons, such that $n_1 + n_2 = n$, in I_b^c' to the 'probability of there being n_i neutrons at time t due to the introduction of a neutron at time $t_o + \Delta t_o$,' for which $i = 1, 2$.

Noting that n_1 and n_2 can be an arbitrary set of combinations, we must actually sum over all those combinations to get the full probability encompassed in the statement. Then by comparing the definition given by Eq. 3.43 with these re-wordings of the events that may occur in I_b^c, we find:

$$\begin{pmatrix}\text{Probability the initial n}^0\text{ collides}\\ \text{in } I_b^c,\text{ resulting in } n \text{ neutrons at } t\end{pmatrix} = P_n(t|t_o+\Delta t_o) \tag{3.47a}$$

$$\begin{pmatrix}\text{Probability those 2 n}^0\text{s produce } n_1 \text{ and}\\ n_2 \text{ n}^0\text{s, such that } n_1+n_2=n, \text{ in } I_b^c\end{pmatrix} = \sum_{n_1+n_2=n} P_{n_1}(t|t_o+\Delta t_o)P_{n_2}(t|t_o+\Delta t_o). \tag{3.47b}$$

For now, we will keep the summation notation that we have written above, but this sum is really a double sum over all possible combinations of n_1 and n_2 that satisfy the condition $n_1+n_2=n$. We will need to keep this in mind later when we are transforming the Master equation to an equation for the probability generating function. Assembling all of the above, we obtain the first collision probability balance for an initial neutron:

$$P_n(t|t_o) = (1-\lambda_f\Delta t_o)P_n(t|t_o+\Delta t_o) + \lambda_f\Delta t_o \sum_{n_1+n_2=n} P_{n_1}(t|t_o+\Delta t_o)P_{n_2}(t|t_o+\Delta t_o). \tag{3.48}$$

Next, we divide by Δt_o and subtract $P_n(t|t_o+\Delta t_o)$ to find:

$$-\frac{P_n(t|t_o+\Delta t_o)-P_n(t|t_o)}{\Delta t_o} = -\lambda_f P_n(t|t_o+\Delta t_o)+\lambda_f \sum_{n_1+n_2=n} P_{n_1}(t|t_o+\Delta t_o)P_{n_2}(t|t_o+\Delta t_o). \tag{3.49}$$

On the left-hand side, we have placed the $P_n(t|t_o+\Delta t_o)$ in front of the $P_n(t|t_o)$ to make the next step easier. If we now evaluate the limit as $\Delta t_o \to 0$, the LHS becomes the derivative of $P_n(t|t_o)$ with respect to t_o, and we thus have:

$$-\frac{\partial P_n(t|t_o)}{\partial t_o} = -\lambda_f P_n(t|t_o) + \lambda_f \sum_{n_1+n_2=n} P_{n_1}(t|t_o)P_{n_2}(t|t_o), \qquad n=0,1,2,\ldots \tag{3.50}$$

which is the backward Master equation for the neutron number distribution due to the introduction of a single neutron at time t_o in a system where the BFM applies. The 'final' condition is:

$$\lim_{t_o\to t} P_n(t|t_o) = \delta_{n,1} \tag{3.51}$$

where $\delta_{i,j}$ is the Kronecker delta function. This condition tells us that as we bring the neutron injection time t_o up to the time of observation t, the probability of there being one neutron in the system is guaranteed.

A difference between this equation and that of the FME, Eq. 3.13 with $S=0$, is that the BME is second-order nonlinear (due to the products $P_{n_1}P_{n_2}$). This nonlinearity has appeared because we need to consider all the possible probabilistic combinations that will result in n neutrons at t due to the two independent chains produced in the IFE in the first collision interval. Something to think about for upcoming chapters: what order of nonlinearity would the BME be if we required j and only j neutrons to be emitted per IFE? (the answer is j-order). Again, we need to keep track of two time quantities: t_o and t because t_o is the operational time variable (i.e., we are taking a derivative with respect to t_o, not t).

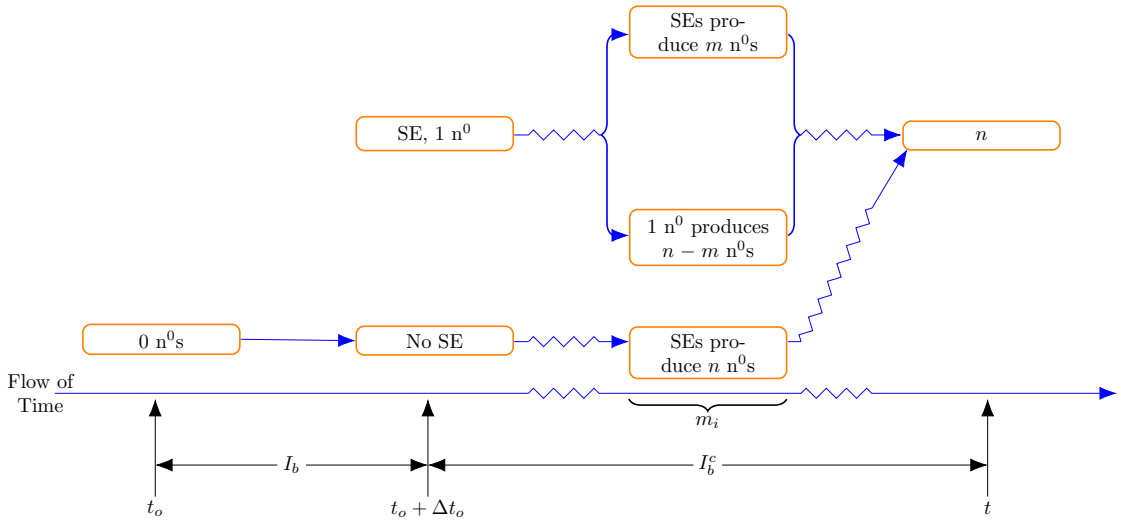


Figure 3.3: Mutually exclusive events that may occur in time interval I_b with their associated states, m_i, that must occur in time interval I_b^c for a singlet-emitting source. SE = Source Event. Note the 'zig-zags' indicate an arbitrary passage of time. If a SE occurs in I_b, producing 1 n^0, then subsequent SEs occurring in I_b^c must produce m n^{0}s and the source n^0 must produce $n-m$ n^{0}s. If no SE occurs in I_b, then subsequent SEs that occur in I_b^c must result in n n^{0}s.

Source

The probability balance and BME derivation for the source case proceeds just as in Chapter 2, Sec. 2.3.1, with the added complexities of neutron induced fission and multiplication. To begin, we define:

$$\Theta_n(t|t_o) = \text{the probability of there existing } n \text{ neutrons within the system at time } t \text{ due to the introduction of a source of strength } S \text{ at an earlier time } t_o. \tag{3.52}$$

Notice this equation is identical to Eq. 2.26, where the difference will be in the physics we incorporate into the RHS.

As we did in Sec. 2.3.1, let us first consider the events that may take place in the first collision interval, from which we will be able to write down a clear probability balance in words. The list of mutually exclusive events that occur in the first collision interval, I_b, are the same as before:

1. No source event occurs
2. A source event occurs, producing 1 neutron.

Note that we assume there are initially zero neutrons within the system and thus no neutron interactions/collisions can occur. Once again, recall Δt_o is sufficiently small such that only one event may occur in Δt_o. We now need to consider the possible pathways stemming from the list above that may lead to the state-space n at time t. In other words, given the two events that may occur in I_b, what consequential events will occur in I_b^c that will lead to n neutrons at t. Using Fig. 3.3, we see that if there is no source event (SE) in I_b, then there must be a collection of source events in

I_b^c that lead to n neutrons at t. If there is a SE, then a single neutron is emitted and we therefore must consider that neutron's progeny (i.e., the neutrons produced in the fission chain) resulting in n_1 neutrons as well as subsequent SEs resulting in $m = n - n_1$ neutrons. Note here that $n = m + n_1$, because if it does not then this particular set of events will not contribute to the LHS of Eq. 3.52.

With this, we may define a probability balance in words:

$$\begin{aligned}\Theta_n(t|t_o) = &\begin{pmatrix}\text{Probability of no SE}\\ \text{occurring in } I_b\end{pmatrix} \times \begin{pmatrix}\text{Probability of subsequent SEs occurring}\\ \text{in } I_b^c \text{ resulting in } n \text{ n}^0\text{s at } t\end{pmatrix}\\ &+ \begin{pmatrix}\text{Probability of 1 SE occurring}\\ \text{in } I_b \text{ producing in 1 n}^0\end{pmatrix} \times \begin{pmatrix}\text{Probability that 1 n}^0 \text{ produces}\\ n_1 \text{ n}^0\text{s in } I_b^c \text{ at } t\end{pmatrix}\\ &\times \begin{pmatrix}\text{Probability of subsequent SEs occurring}\\ \text{in } I_b^c \text{ resulting in } n - n_1 \text{ n}^0\text{s at } t\end{pmatrix}.\end{aligned} \tag{3.53}$$

Just as before, we can easily define the probability of a source event occurring in the short time Δt_o by recalling that the source, S, is defined as 'the probability of a source event occurring per unit time', which results in the following:

$$\begin{pmatrix}\text{Probability of 1 SE occurring}\\ \text{in } I_b \text{ producing in 1 n}^0\end{pmatrix} = S\Delta t_o \tag{3.54}$$

Next, we may define the complement of Eq. 2.29 using the conservation of probability to find:

$$\begin{pmatrix}\text{Probability of no SE}\\ \text{occurring in } I_b\end{pmatrix} = 1 - S\Delta t_o \tag{3.55}$$

Next, we need not consider explicit, singular events that may occur in I_b^c to write the subsequent probabilities. Let us first consider the 'probability of subsequent SEs occurring in I_b^c resulting in n n^{0}s at t,' by changing the wording to the 'probability of there being n neutrons at time t due to the introduction of a source at time $t_o + \Delta t_o$,' which is simply equivalent to $\Theta_n(t|t_o + \Delta t_o)$. We may make this equivalence because each source event is independent of all other source events. Similarly, let us alter the 'probability of subsequent source events occurring in I_b^c resulting in $m = n - n_1$ neutrons at t' to the 'probability of there being $m = n - n_1$ neutrons at time t due to the introduction of a source at time $t_o + \Delta t_o$,' which is $\Theta_m(t|t_o + \Delta t_o)$. Finally, we change the 'probability the 1 neutron produces n_1 neutrons in I_b^c at t' to the 'probability of there being n_1 neutrons at t due to the introduction of a single neutron at time $t_o + \Delta t_o$,' which is $P_{n_1}(t|t_o + \Delta t_o)$. Now, because m and n_1 are arbitrary, we must sum over all combinations of $m + n_1$ that satisfy the condition $m + n_1 = n$, which we write colloquially as: $\sum_{m+n_1=n}()$.

Assembling these together, we obtain the first collision probability balance for a singlet-emitting neutron source in an infinite medium with no capture and binary fission:

$$\Theta_n(t|t_o) = (1 - S\Delta t_o)\Theta_n(t|t_o + \Delta t_o) + S\Delta t_o \sum_{m+n_1=n} \Theta_m(t|t_o + \Delta t_o)P_{n_1}(t|t_o + \Delta t_o). \tag{3.56}$$

Next, we divide by Δt_o and subtract $\Theta_n(t|t_o + \Delta t_o)$ to find:

$$-\frac{\Theta_n(t|t_o + \Delta t_o) - \Theta_n(t|t_o)}{\Delta t_o} = -S\Theta_n(t|t_o + \Delta t_o) + S \sum_{m+n_1=n} \Theta_m(t|t_o + \Delta t_o)P_{n_1}(t|t_o + \Delta t_o). \tag{3.57}$$

If we now evaluate the limit as $\Delta t_o \to 0$, the LHS becomes the derivative of $\Theta_n(t|t_o)$ with respect to t_o, and we have:

$$-\frac{\partial \Theta_n(t|t_o)}{\partial t_o} = -S\Theta_n(t|t_o) + S \sum_{m+n_1=n} \Theta_m(t|t_o)P_{n_1}(t|t_o), \qquad n = 0, 1, 2, \ldots \tag{3.58}$$

which is the backward Master equation for the neutron number distribution in the presence of a singlet-emitting neutron source in an infinite medium with the binary fission model and no capture. The 'final' condition, for which there are zero neutrons in the system at time t_o, is given by

$$\lim_{t_o \to t} \Theta_n(t|t_o) = \delta_{n,0} \tag{3.59}$$

where $\delta_{i,j}$ is the Kronecker delta function.

As with the single chain case, we see Eq. 3.58 is substantially more complex than the radioactive decay BME, Eq. 2.34. With the inclusion of neutron interactions, we see that the source BME is a function of the solution to the single chain BME, $P_n(t|t_o)$. This dependence arose because we require knowledge of the single chain that is initiated by the source event that occurs in the first collision interval. As a preliminary thought, what might we expect the equation to look like if we allowed for j neutrons to be emitted after that I_b source event? (answer: we would then need to account for each chain's population, $n_1, n_2, \ldots, n_j$, at time t that sum to n with subsequent source event contributions accounted for as well).

3.3.2 Equations for the Probability Generating Function

We now transform the BMEs, given by Eqs. 3.50 and 3.58, using the probability generating functions (PGFs).

Single Chain

We now transform the infinite set of differential-difference equations given by Eq. 3.50 into a single PDE satisfied by the probability generating function (PGF), defined as:

$$G(z,t|t_o) = \sum_{n=0}^{\infty} z^n P_n(t|t_o). \tag{3.60}$$

The transformation is facilitated by multiplying Eq. 3.50 by z^n and summing over all n to find:

$$-\sum_{n=0}^{\infty} z^n \frac{\partial P_n(t|t_o)}{\partial t_o} = -\lambda_f \sum_{n=0}^{\infty} z^n P_n(t|t_o) + \lambda_f \sum_{n=0}^{\infty} z^n \sum_{n_1+n_2=n} P_{n_1}(t|t_o) P_{n_2}(t|t_o). \tag{3.61}$$

The LHS is simply $-\partial G/\partial t_o$ and the first term on the RHS is $-\lambda_f G$. The combinatorial sum on the RHS is converted as follows:

$$\begin{aligned} \mathcal{I}_2(z,t|t_o) &= \sum_{n=0}^{\infty} z^n \sum_{n_1+n_2=n} P_{n_1}(t|t_o) P_{n_2}(t|t_o) \\ &= \sum_{n=0}^{\infty} z^n \sum_{n_1=0}^{\infty} P_{n_1} \sum_{n_2=0}^{\infty} P_{n_2}, \qquad n_1+n_2=n \\ &= \sum_{n_1=0}^{\infty} P_{n_1} \sum_{n=0}^{\infty} z^n P_{n-n_1}. \end{aligned} \tag{3.62}$$

In the second line, we explicitly allow for n_1 and n_2 to sum to infinity such that the only contributing (non-zero) terms are the terms that satisfy the explicit condition $n_1 + n_2 = n$. In going from the second to third line, we have restricted values of n_2 to be those that satisfy $n_2 = n - n_1$ and thus

the sum over n_2 vanishes because there is only one value of n_2 which satisfies $n_2 = n - n_1$ for a given n_1. Next, define the index $j = n - n_1$, then $n = j + n_1$ and $z^n = z^j z^{n_1}$. Noting that when $n = 0$, $j = -n_1$ and since $P_{-n_1} = 0$, we may start the sum at $j = 0$, we find:

$$\begin{aligned}\mathcal{I}_2(z,t|t_o) &= \sum_{n_1=0}^{\infty} z^{n_1} P_{n_1}(t|t_o) \sum_{j=0}^{\infty} z^j P_j(t|t_o) \\ &= G(z,t|t_o)G(z,t|t_o) \\ &= \big[G(z,t|t_o)\big]^2.\end{aligned} \tag{3.63}$$

where we note that, going from the first to the second line, the sums are completely decoupled from one another and we therefore obtain a simple product of the PGF.

Assembling the transformations yields the single chain PGF PDE:

$$-\frac{\partial G(z,t|t_o)}{\partial t_o} = -\lambda_f G(z,t|t_o) + \lambda_f \big[G(z,t|t_o)\big]^2 \tag{3.64}$$

with final condition given by:

$$\lim_{t_o \to t} G(z,t|t_o) = z. \tag{3.65}$$

This PGF PDE for the single chain is a first-order quadratically nonlinear PDE which can be solved with the Method of Characteristics.

Comparing Eq. 3.64 with the single chain forward version of Eq. 3.21 (set $S = 0$), we see some big differences between the forward and backward equations. First, the backward equation does not have a $\partial G / \partial z$ term while the forward equation does. Also, the forward equation is linear while the backward equation is nonlinear due to the G^2 term. We also note that, aside from the initial and final conditions (which are functionally the same), the backward equation does not have any explicit z dependence while the forward equation has the variable coefficient $\lambda_f(z^2 - z)$. It is interesting that the forward equation has a z^2 while the backward case has a G^2 appearing the respective equations. The resemblance between Eq. 3.64 and the characteristic equation 3.24a demonstrates that, aside from the direction of time, these two equations are providing the same information about the single chain probabilistic propagation mechanics. On a final note, the backward equation has a negative time derivative (i.e., an adjoint time derivative) and when we attempt to solve it, we will need to integrate backwards in time.

Source

The probability generating function (PGF) for the source case is defined as:

$$H(z,t|t_o) = \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o), \tag{3.66}$$

where we intentionally use a different symbol from the single chain PGF, G. The transform variable, z, is a real number with domain: $z \in [0,1]$, which ensures absolute convergence.

We may transform the BME given by Eq. 3.58 by multiplying the equation by z^n and summing over all n to find:

$$-\sum_{n=0}^{\infty} z^n \frac{\partial \Theta_n(t|t_o)}{\partial t_o} = -S \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o) + S \sum_{n=0}^{\infty} z^n \sum_{m+n_1=n} \Theta_m(t|t_o) P_{n_1}(t|t_o). \tag{3.67}$$

We may immediately see that the LHS becomes $-\partial H/\partial t_o$ and the first term on the RHS becomes $-SH$. Let us take special care to analyze the combinatorial sum, I_1^S, where the subscript denotes the number of neutrons emitted per source event:

$$\begin{aligned}\mathcal{I}_1^S(z,t|t_o) &= \sum_{n=0}^{\infty} z^n \sum_{m+n_1=n} \Theta_m(t|t_o) P_{n_1}(t|t_o) \\ &= \sum_{n=0}^{\infty} z^n \sum_{m=0}^{\infty} \Theta_m \sum_{n_1=0}^{\infty} P_{n_1}, \qquad m+n_1=n \\ &= \sum_{m=0}^{\infty} \Theta_m \sum_{n=0}^{\infty} z^n P_{n-m}.\end{aligned} \tag{3.68}$$

In the second line, we explicitly allow for m and n_1 to sum to infinity such that the only contributing (non-zero) terms are the terms that satisfy the explicit condition $m+n_1=n$. In going from the second to third line, we have restricted values of n_1 to be those that satisfy $n_1=n-m$ and thus the sum over n_1 vanishes because there is only one value of n_1 which satisfies $n_1=n-m$ for a given m. Next, define the index $j=n-m$, then $n=j+m$ and $z^n=z^j z^m$. Noting that when $n=0$, $j=-m$ and since $P_{-m}=0$, we may start the sum at $j=0$, we find:

$$\begin{aligned}\mathcal{I}_1^S(z,t|t_o) &= \sum_{m=0}^{\infty} z^m \Theta_m(t|t_o) \sum_{j=0}^{\infty} z^j P_j(t|t_o) \\ &= H(z,t|t_o) G(z,t|t_o).\end{aligned} \tag{3.69}$$

where we note that, going from the first to the second line, the sums are completely decoupled from one another and we therefore obtain a simple product of the single chain and source PGFs.

Assembling the transformed quantities, we obtain a PDE for the source PGF:

$$-\frac{\partial H(z,t|t_o)}{\partial t_o} = -SH(z,t|t_o) + SH(z,t|t_o)G(z,t|t_o) \tag{3.70}$$

with the final condition

$$\lim_{t_o \to t} H(z,t|t_o) = 1. \tag{3.71}$$

This equation is easily solved via separation of variables and then integration backwards in time.

3.3.3 Solution to the PGF PDE

Single Chain

We now aim to solve Eq. 3.64 for G using the Method of Characteristics. Noting the total derivative of G with respect to t_o is:

$$\frac{\mathrm{d}G}{\mathrm{d}t_o} = \frac{\partial G}{\partial t_o} + \frac{\partial G}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t_o}, \tag{3.72}$$

from which we obtain the following system of ODEs:

$$\frac{\mathrm{d}z}{\mathrm{d}t_o} = 0 \tag{3.73a}$$

$$\frac{\mathrm{d}G}{\mathrm{d}t_o} = \lambda_f G - \lambda_f G^2. \tag{3.73b}$$

Equation 3.73a informs us that z is a constant and Eq. 3.73b is a Riccati equation which can be solved by linearizing with the variable $w = 1/G$ and then solved with the integrating factor. Solving the linear equation in w, reverting back to G, and using the final condition, Eq. 3.65, yields:

$$G(z,t|t_o) = \left[1 + \frac{1-z}{z}\mathrm{e}^{-\lambda_f(t-t_o)}\right]^{-1} \tag{3.74}$$

which can be rearranged as:

$$G(z,t|t_o) = \frac{z\mathrm{e}^{-\lambda_f(t-t_o)}}{1-z[1-\mathrm{e}^{-\lambda_f(t-t_o)}]} \tag{3.75}$$

which is exactly equivalent to Eq. 3.31, the forward single chain solution.

Source

To find the system of characteristic ODEs, let us consider the total derivative of H:

$$\frac{\mathrm{d}H}{\mathrm{d}t_o} = \frac{\partial H}{\partial t_o} + \frac{\partial H}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t_o}. \tag{3.76}$$

Comparing this equation to the BME given by Eq. 3.70, we may infer the system of ODEs as:

$$\frac{\mathrm{d}z}{\mathrm{d}t_o} = 0 \tag{3.77a}$$

$$\frac{\mathrm{d}H}{\mathrm{d}t_o} = SH(-1+G). \tag{3.77b}$$

Again, Eq. 3.77a informs us that z is a constant and Eq. 3.77b is a first-order separable ODE. Inserting Eq. 3.75 into Eq. 3.77b, separating and integrating provides:

$$\int_{H(z,t|t)}^{H(z,t|t_o)} \frac{\mathrm{d}H}{H} = S\int_t^{t_o} \mathrm{d}t_o' \left[1 + \frac{z}{1-z}\mathrm{e}^{-\lambda_f(t-t_o')}\right]^{-1}. \tag{3.78}$$

Recalling the final condition $H(z,t|t) = 1$, the above is solved:

$$\ln\left[H(z,t|t_o)\right] = -S(t-t_o) + \frac{S}{\lambda_f}\ln\left[\frac{1}{1-z\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)}\right]. \tag{3.79}$$

Solving for H yields the solution:

$$H(z,t|t_o) = \mathrm{e}^{-S(t-t_o)}\left[1 - z\left(1-\mathrm{e}^{-\lambda_f(t-t_o)}\right)\right]^{-\eta}, \tag{3.80}$$

where η is defined by Eq. 3.38, replicated here for convenience:

$$\eta = \frac{S}{\lambda_f}. \tag{3.81}$$

Note that Eq. 3.80 is identical to the forward formulation counterpart, Eq. 3.34.

The next step will be to find the number distribution using this solution, shown in the next section.

3.3.4 Inversion of the PGF

Since the PGF solutions for the forward and backward case are identical, the following is the same as what is presented in Sec. 3.2.4. We replicate the process below in the spirit of completion and to reinforce the process.

Single Chain

We aim to invert Eq. 3.75, which can be done by rearranging and Taylor expanding about $z = 0$:

$$\begin{aligned} G(z,t|t_o) &= z\mathrm{e}^{-\lambda_f(t-t_o)}\left[1 - z\left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)\right]^{-1} \\ &= z\mathrm{e}^{-\lambda_f(t-t_o)}\sum_{n=0}^{\infty}\left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)^n z^n \end{aligned} \tag{3.82}$$

where we note that this expansion is convergent because the quantity $(1 - \mathrm{e}^{-\lambda_f(t-t_o)})$ is always bounded between 0 and 1 and therefore the entire bracketed quantity on the first line of Eq. 3.82 is also bounded between 0 and 1 for all t and all $z \in [0,1]$. Let us absorb the z in the front of the expression of Eq. 3.82 into the sum, define the index $m = n + 1$ (and rename the index $m \to n$) to find:

$$G(z,t|t_o) = \mathrm{e}^{-\lambda_f(t-t_o)}\sum_{n=1}^{\infty}\left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)^{n-1} z^n \tag{3.83}$$

By now comparing Eq. 3.83 with the original definition of the PGF: $G(z,t|t_o) = \sum_{n=0}^{\infty} z^n P_n(t|t_o)$, we may extract the neutron number PDF for a single chain to find:

$$P_n(t|t_o) = \mathrm{e}^{-\lambda_f(t-t_o)}\left[1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right]^{n-1} \tag{3.84}$$

for $n = 1, 2, 3, \ldots$. Note that the value for $n = 0$ is $P_0(t) = 0$ because we have a single initial neutron that can only induce fissions, thus the chain will not die away because we have not allowed for any mechanism to do so. We may also verify the initial condition by setting $t = t_o$ to find $P_n(t_o) = \delta_{n,1} = 0^{n-1}$. Thus, 0^{n-1} is equal to 0 except when $n = 1$, whence $0^0 = 1$, proving the initial condition is satisfied.

Singlet-Emitting Source Solution

Equation 3.80 may be Taylor expanded about $z = 0$ to yield:

$$\begin{aligned} H(z,t|t_o) &= \mathrm{e}^{-S(t-t_o)}\left[1 - z\left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)\right]^{-\eta} \\ &= \mathrm{e}^{-S(t-t_o)}\sum_{n=0}^{\infty}\frac{\eta(\eta+1)\cdots(\eta+n-1)}{n!}\left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)^n z^n. \end{aligned} \tag{3.85}$$

This series is convergent for the same reasons described in the single chain inversion section above. Once again, if we compare the above expression with the original definition of the PGF: $H(z,t|t_o) = \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o)$, we find the neutron number distribution in the presence of a singlet-emitting source. Noting the identity:

$$\eta(\eta+1)\cdots(\eta+n-1) = \frac{\Gamma(\eta+n)}{\Gamma(\eta)}, \tag{3.86}$$

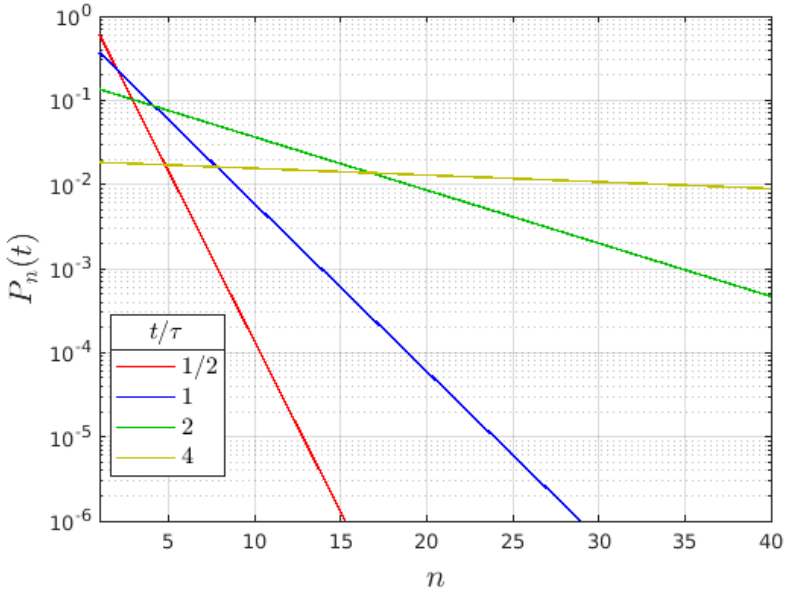


Figure 3.4: Neutron number distributions for a single chain in a system that follows the BFM without capture.

where $\Gamma(\cdot)$ is the gamma function, the number distribution is stated as:

$$\Theta_n(t|t_o) = \mathrm{e}^{-S(t-t_o)} \frac{\Gamma(\eta+n)}{n!\Gamma(\eta)} \left(1 - \mathrm{e}^{-\lambda_f(t-t_o)}\right)^n. \tag{3.87}$$

We may verify the final condition, $\Theta_n(t|t) = \delta_{n,0}$, by setting $t = t_o$ to find $\Theta_n(t|t) = \Gamma(\eta + n)/(n!\Gamma(\eta))0^n$. Thus, 0^n is only non-zero when $n = 0$, whence $0^0 = 1$- verifying the final condition.

3.4 Examples & Discussion

Consider the system where there is no capture, $\sigma_c = 0\ b$, and therefore every time a neutron collides with a nucleus, an induced fission event occurs and we have $p_f = \sigma_f/(\sigma_f + \sigma_c) = 1$ (from Eq. 1.8). Following every collision, exactly two neutrons are emitted ($q_\nu^f = \delta_{\nu,2}$- the BFM) and therefore $\overline{\nu} = 2$ and $k = \overline{\nu} p_f = 2$ (from Eq. 1.7). Although a neutron is lost in the absorption process, two neutrons emerge and we technically do not have a loss mechanism within the model still; therefore it is expected that the neutron chain will not (and cannot) perish. This is further expressed in Eq. 3.37 (and Eq. 3.84), where we explicitly cannot set $n = 0$ in that equation. We have calculated the neutron number distribution due to a single initial neutron for this system using Eq. 3.37 (or Eq. 3.84), shown in Fig. 3.4. For this system, we are assuming the neutrons are fast (14 MeV) and thus have a velocity of $v = 5.174 \cdot 10^9\ cm/s$. The system is composed of pure ^{235}U metal and useful data can be found in Table 3.1.

Figure 3.4 shows the number distribution due to a single neutron that is introduced at time $t_o = 0\ s$ at several later times t (scaled by the neutron lifetime, τ). As mentioned above, there is no loss mechanism and therefore the chain's population will only grow as time progresses and

Table 3.1: Data for a ^{235}U system that follows the BFM without capture.

$N\ [b^{-1}cm^{-1}]$	$\sigma_f\ [b]$	$\sigma_c\ [b]$	$\overline{\nu}$	$v\ [cm/s]$	$\tau\ [ns]$	$\lambda_f\ [1/s]$
0.05088	2.053	0	2	$5.174 \cdot 10^9$	1.8501	$5.4050 \cdot 10^8$

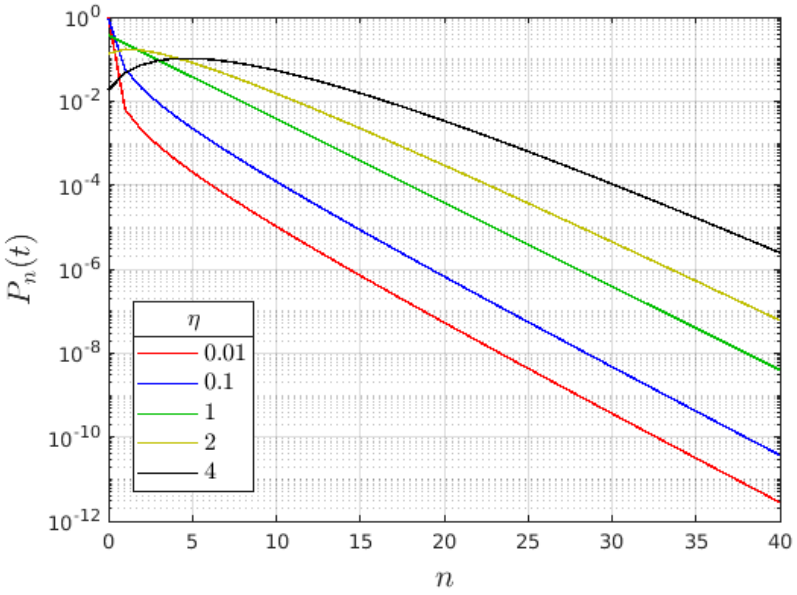


Figure 3.5: Neutron number distributions due to a singlet-emitting source in a system that follows the BFM without capture.

more generations of neutrons are produced. Noting that the horizontal axis starts at $n = 1$, we see this ever-growing behavior expressed as a reduction of P_1 as time progresses, telling us that the probability that the initial neutron has not collided and induced a fission is exponentially decaying in time. As P_1 decreases, the distribution's mass moves toward the right (toward ∞) and appears to 'flatten'. This flattening is accompanied by an overall reduction in the magnitude of the distribution (although it is still normalized) because the neutron population is moving outward toward ∞ with certainty. If we evaluated the limit as $t \to \infty$ of Eq. 3.37, we would find $\lim_{t\to\infty} P_n(t) = 0$ for all $n \in \mathbb{R}$. This must be interpreted with caution, as we know the chain's population is always growing and there must then be a value of n that satisfies the normalization condition as well as our intuition. That value is $n = \infty$, which tells us that in the infinite future, we will have an infinite number of neutrons within the system with probability $P_\infty(\infty) = 1$.

We now consider the case where the above ^{235}U system has a singlet-emitting neutron source at a given time of $t = \tau$. Figure 3.5 shows the neutron number distribution due to several sources of varying strength where we have expressed the magnitude of the source strength in terms of η, Bell's parameter, which is defined by Eq. 3.38 for the BFM. For convenience, we state it here: $\eta = S/\lambda_f$, which is essentially the ratio of the source rate to the induced fission rate and is a measure of the two competing neutron production mechanisms. As we see in Fig. 3.5, the larger η (corresponding to

larger S relative to a constant λ_f), the lower the probability of finding zero neutrons in the system at a given time. This agrees with our intuition, which is to expect P_0 to be lessened as the probability of a source event per unit time is increased. An additional feature worth noting is that the distribution undergoes a qualitative change from a monotonically decreasing distribution for $\eta < 1$ to a unimodal distribution when $\eta > 1$. This is again due to the decrease of P_0 for increasing S which then moves the mass of the distribution to larger populations. Thus, a system with $\eta < 1$ will have a number distribution that is characteristically similar to the exponentially decreasing single chain distribution and tells us that λ_f dominates over S. For a system with $\eta > 1$, the source events are more closely spaced in time and the fission chains produced in source events will overlap, causing a building-up effect about a centralized mean value (this is what causes the shift to a unimodal distribution due to the decreasing likelihood of there being 0 neutrons in the system as time progresses).

Chapter 4

Full Multiplicity for Induced Fission and Sources

In this chapter, we expand the model from the previous chapter to allow for more realistic physics including neutron capture, neutron leakage, and multiplicity distributions for both induced fission and source events. This will bring the reader to the forefront of being able to read classic papers, such as Bell's from 1963, as well as to write their own master equations and apply the MESA to attempt to solve them. At the end of the chapter, we will include a discussion of the NMESA branch of the MESA (the right column seen in Fig. 1.5) to give the reader a taste of a more practical solution method and to hedge the effectiveness of certain approximations we will apply in the MESA of this "full multiplicity" model.

4.1 The Model

The model for this chapter includes the following new physics:

- neutron capture (often called radiative capture or parasitic capture),
- neutron leakage from the system,
- full multiplicity distributions for induced fission events and source events.

We will see that these master equations are not outright solvable due to the full multiplicity distributions. The issue will become apparent, in the forward case, when we attempt to solve the PGF PDE using the Method of Characteristics. Similarly, we will hit a roadblock in the backward case when trying to compute integrals showing up in the PGF solution process for both the single chain and source equations. When we need to solve the single chain (forward and backward) cases, we will make an approximation to the fission multiplicity distribution PGF (which we have not seen explicitly yet) that will allow us to evaluate an integral. This approximation is called the *Quadratic Approximation* and was first devised by Bell [9]. For the source cases, we will assume that the source emits a single neutron per event. In both of these assumptions, we will see how well they hold compared to reality, which tends to be relatively accurate for certain types of reactors.

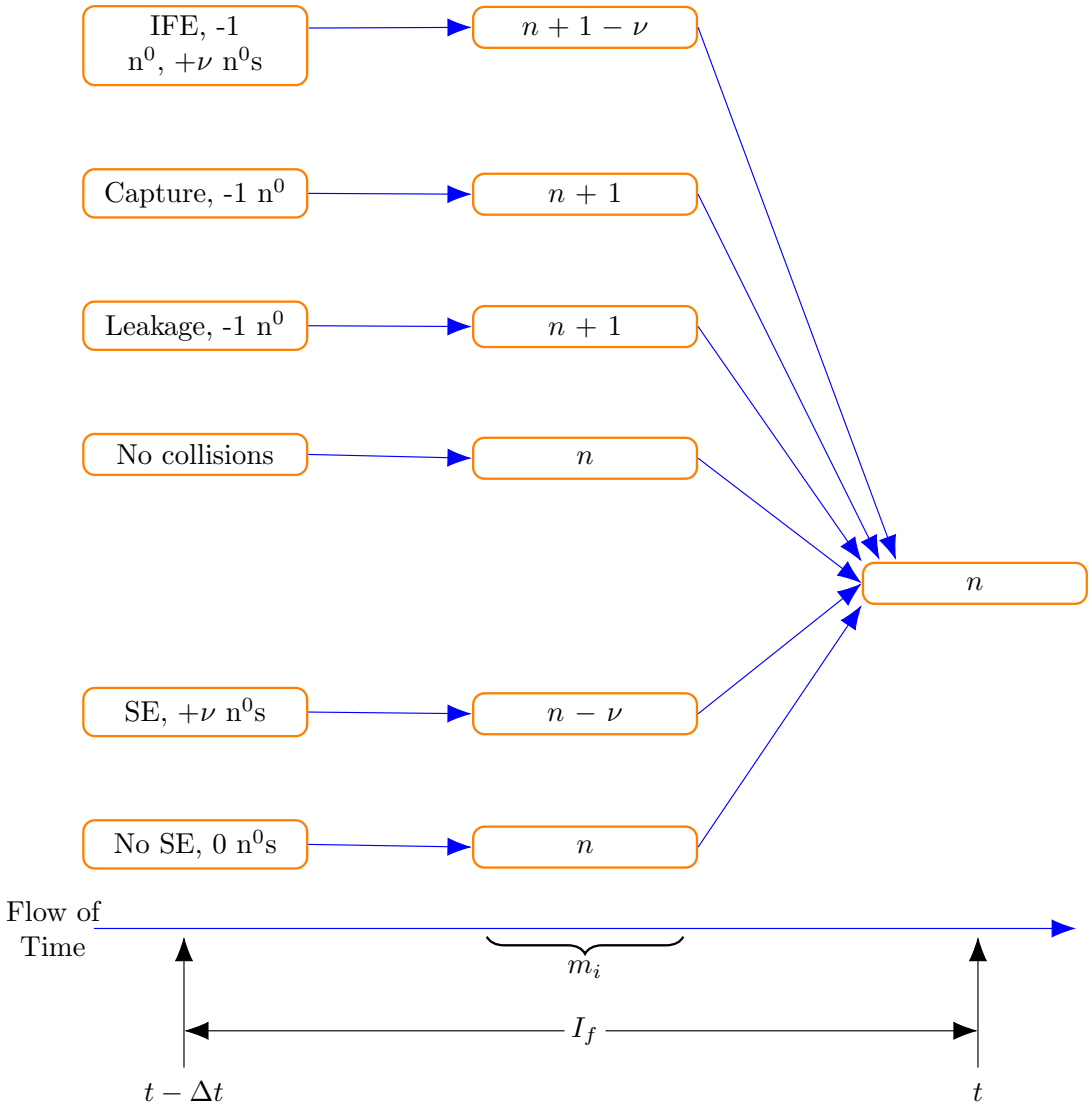


Figure 4.1: Forward formulation event tree for full induced fission and source multiplicity distributions. Here $\nu = 0, 1, \ldots, \nu_m^x$, where $x = \{f, S\}$ for IFEs and SEs, respectively, and ν_m^x is the maximum number of neutrons emitted per event of type-x.

4.2 Forward Formulation

4.2.1 Probability Balance & Master Equation

As before, we define the probabilistic quantity we wish to calculate:

$$P_n(t) = \text{the probability of there existing } n \text{ neutrons within the system at time } t. \tag{4.1}$$

This definition is the same as Eq. 3.1, but we will need to account for the many new physical interactions that may occur to the neutron population in the last collision interval.

To determine $P_n(t)$, we use knowledge of the possible states the system could be occupying a short time before t, given by $t - \Delta t$, and probability balance is conducted over the time domain:

$$I_f = [t - \Delta t, t], \tag{4.2}$$

where the subscript f refers to this being the forward time interval. We assume Δt is sufficiently small enough that only a single source event or neutron collision may reasonably occur within it. In constructing the probability balance, let us first state the possible events that may occur within the short time interval I_f:

1. a neutron collides and is absorbed, causes an induced fission event (IFE), and ν neutrons are emitted, where $\nu = 0, 1, \ldots, \nu_m^f$ and ν_m^f is the maximum number or neutrons emitted per IFE,
2. a source event occurs, emitting ν neutrons where $\nu = 0, 1, \ldots, \nu_m^S$ and ν_m^S is the maximum number or neutrons emitted per SE,
3. a neutron collides and is captured,
4. a neutron leaks out of the system,
5. no event occurs (no neutrons collide with nuclei and no source events occur)

The event tree in Fig. 4.1 shows this list in action. In the figure, we see the event that may occur in the far-left bubbles with the resultant number of neutrons that emerge, followed by the intermediary state m_i- the i^{th} state that is connected to state n. Using the list above along with Fig. 4.1, we write the probability balance in words as follows:

$$\begin{aligned}
P_n(t) = &\left(\begin{array}{c}\text{Probability of no source}\\ \text{event occurring in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability that none of}\\ \text{the } n \text{ n}^0\text{s collide in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in}\\ \text{state } n \text{ at time } t - \Delta t\end{array}\right) \\
&+ \left[\left(\begin{array}{c}\text{Probability that 1 n}^0\\ \text{is captured in } I_f\end{array}\right) + \left(\begin{array}{c}\text{Probability that 1 n}^0\\ \text{leaks in } I_f\end{array}\right)\right] \times \left(\begin{array}{c}\text{Probability of being in state}\\ n+1 \text{ at time } t - \Delta t\end{array}\right) \\
&+ \left(\begin{array}{c}\text{Probability of 1 source}\\ \text{event occurring in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of 0 n}^0\text{s}\\ \text{being emitted}\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in state}\\ n \text{ at time } t - \Delta t\end{array}\right) \\
&+ \left(\begin{array}{c}\text{Probability of 1 source}\\ \text{event occurring in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of 1 n}^0\\ \text{being emitted}\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in state}\\ n-1 \text{ at time } t - \Delta t\end{array}\right) \\
&\vdots \\
&+ \left(\begin{array}{c}\text{Probability of 1 source}\\ \text{event occurring in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of } \nu_m^S \text{ n}^0\text{s}\\ \text{being emitted}\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in state}\\ n - \nu_m^S \text{ at time } t - \Delta t\end{array}\right) \\
&+ \left(\begin{array}{c}\text{Probability of 1 n}^0\\ \text{causing an IFE in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of 0 n}^0\text{s}\\ \text{being emitted}\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in state}\\ n-1 \text{ at time } t - \Delta t\end{array}\right) \\
&+ \left(\begin{array}{c}\text{Probability of 1 n}^0\\ \text{causing an IFE in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of 1 n}^0\\ \text{being emitted}\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in state}\\ n \text{ at time } t - \Delta t\end{array}\right) \\
&\vdots \\
&+ \left(\begin{array}{c}\text{Probability of 1 n}^0\\ \text{causing an IFE in } I_f\end{array}\right) \times \left(\begin{array}{c}\text{Probability of } \nu_m^f \text{ n}^0\text{s}\\ \text{being emitted}\end{array}\right) \times \left(\begin{array}{c}\text{Probability of being in state}\\ n+1-\nu_m^f \text{ at time } t - \Delta t\end{array}\right)
\end{aligned} \tag{4.3}$$

The first line concerns the probability that no event occurs and appears the same as the previous version, Eq. 3.3 (we will have a different total reaction rate now, however). The second line shows the capture and leakage events, where we note that we grouped the capture and leakage probabilities together because they have the same intermediary state, $m_i = n + 1$. From the population balance perspective, it does not matter which process causes the loss of one neutron (remember the Markov property) just as long as we are in state $n + 1$, then lose 1 neutron, which takes the system to state n. We have written the source emission probabilities out to make it clear that each neutron number emission following a SE has a different connected state. The reasoning is as follows: following a SE, ν neutrons are born and thus the system gains ν neutrons. Thus the, system needs to be in state $n - \nu$ is order for the $+\nu$ to cancel and bring the system to state n. For the IFE case, we must also consider the loss of the neutron that causes the IFE by being absorbed into the nucleus it collides with. Once that neutron is absorbed we then must account for the gain of ν neutrons following the IFE. Notice how each event from the above list is multiplied by a connected (dependent) probabilistic state. These connected states have already been defined for us with Eq. 4.1 where we need only change the index and time argument to fix the description.

We may now start defining the probabilities to convert the probability balance from words to math. We will walk through the same process as we did in the previous chapters so as to provide a full walkthrough. Let us start with the source probabilities. The source, S, should be thought of as "the probability of a source event occurring per unit time", and thus we may define the probability of a source event occurring in the time interval Δt as:

$$\left(\begin{array}{c} \text{Probability of 1 source} \\ \text{event occurring in } I_f \end{array} \right) = S(t - \Delta t)\Delta t, \tag{4.4}$$

where we are now allowing the source to be time-dependent and we must consider the source strength at the beginning of I_f. From Eq. 4.4 and keeping in mind that Δt is sufficiently small, we may utilize the conservation of probability to determine:

$$\left(\begin{array}{c} \text{Probability of no source} \\ \text{event occurring in } I_f \end{array} \right) = 1 - S(t - \Delta t)\Delta t. \tag{4.5}$$

Next, we need to determine the probability that a neutron reacts in some manner. Recall that the reaction rate of interaction x, λ_x, can be thought of as the "probability that event type x occurs per unit time per neutron." We note that this includes the two new processes of capture and leakage which have reactions rates λ_c and λ_ℓ. Thus, for a single neutron propagating in the time interval Δt, we have:

$$\begin{aligned} \left(\begin{array}{c} \text{Probability that 1} \\ \text{n}^0 \text{ interacts in } I_f \end{array} \right) &= \Big[\lambda_c(t - \Delta t) + \lambda_\ell(t - \Delta t) + \lambda_f(t - \Delta t)\Big]\Delta t \\ &= \lambda_t(t - \Delta t)\Delta t, \end{aligned} \tag{4.6}$$

where we have defined the total reaction rate:

$$\lambda_t = \lambda_c + \lambda_\ell + \lambda_f. \tag{4.7}$$

We include the leakage rate as part of the total reaction rate because it is a rate that is dependent on the neutron population present within the system and it also causes a change in the population upon the event occurring. Similar to how we arrived at Eq. 4.5, we use the conservation of probability to determine the probability that one neutron does not interact in I_f as: $1 - \lambda_t\Delta t$. Notice that that expression is for a *single* neutron, and we therefore need to multiply $1 - \lambda_t\Delta t$ to itself for each

neutron present in the system. If no collisions/leakages have occurred in Δt, then there must already be n neutrons in the system at $t - \Delta t$. From this, we find:

$$\left(\begin{array}{c} \text{Probability that none of the} \\ n \text{ n}^0\text{s collide/leak in } I_f \end{array} \right) = \Big[1 - \lambda_t(t - \Delta t)\Delta t\Big]^n. \tag{4.8}$$

Following that same multiplicative process, if we want to know the probability that 1 neutron is captured or leaks from the system of the $n + 1$ neutrons present, we may write:

$$\left(\begin{array}{c} \text{Probability that 1 of the } n+1 \\ \text{n}^0\text{s is captured or leaked in } I_f \end{array} \right) = (n+1)\Big[\lambda_c(t - \Delta t) + \lambda_\ell(t - \Delta t)\Big]\Delta t. \tag{4.9}$$

Similarly, the induced fission reaction rate may be calculated for the $n + 1 - \nu$ neutrons that are present before the IFE occurs in Δt:

$$\left(\begin{array}{c} \text{Probability of } n+1-\nu \\ \text{n}^0\text{s causing an IFE in } I_f \end{array} \right) = (n + 1 - \nu)\lambda_f(t - \Delta t)\Delta t. \tag{4.10}$$

For the SE and IFE multiplicity distributions, we simply need to recall that the probability of ν neutrons being emitted following event type x is an experimentally derived quantity and can be expressed simply as:

$$\left(\begin{array}{c} \text{Probability of } \nu \text{ n}^0\text{s being} \\ \text{emitted from event type } x \end{array} \right) = q_\nu^x. \tag{4.11}$$

Now let us address the connected state probabilities of Eq. 4.3. The first one is the "probability of being in state n at time $t - \Delta t$", and by comparing that statement to Eq. 4.1, we find that that is equivalent to the quantity $P_n(t - \Delta t)$. The connected state for the capture and leakage probabilities is $P_{n+1}(t - \Delta t)$ and the SE and IFE connected states follow in the same manner.

Assembling these connected states with Eqs. 4.4 through 4.11, we may write down the probability balance for the full multiplicity model with capture and leakage:

$$\begin{aligned} P_n(t) = &\Big[1 - S(t - \Delta t)\Delta t\Big]\Big[1 - \lambda_t(t - \Delta t)\Delta t\Big]^n P_n(t - \Delta t) \\ &+ (n+1)\Big[\lambda_c(t - \Delta t) + \lambda_\ell(t - \Delta t)\Big]\Delta t P_{n+1}(t - \Delta t) \\ &+ S(t - \Delta t)\Delta t \sum_{\nu=0}^{\nu_m^S} q_\nu^S P_{n-\nu}(t - \Delta t) \\ &+ \lambda_f(t - \Delta t)\Delta t \sum_{\nu=0}^{\nu_m^f} q_\nu^f (n + 1 - \nu) P_{n+1-\nu}(t - \Delta t). \end{aligned} \tag{4.12}$$

We have consolidated all the SE and IFE emission probabilities into their respective sums.

Before continuing, we may rewrite the "no event" probability by expanding $(1 - \lambda_t\Delta t)^n$ in a Taylor series about $\lambda_t\Delta t = 0$ (suppressing time-dependence for brevity):

$$\begin{aligned} (1 - \lambda_t\Delta t)^n =& 1 - n\lambda_t\Delta t + \frac{1}{2}n(n-1)\left(\lambda_t\Delta t\right)^2 - \frac{1}{6}n(n-1)(n-2)\left(\lambda_t\Delta t\right)^3 + \cdots \\ =& 1 - n\lambda_t\Delta t + \mathcal{O}\left([\Delta t]^2\right), \end{aligned} \tag{4.13}$$

where $\mathcal{O}$ is the Big-O notation. We may then write:

$$\Big[1 - S(t - \Delta t)\Delta t\Big]\Big[1 - \lambda_t(t - \Delta t)\Delta t\Big]^n = 1 - \Big[S(t - \Delta t) + n\lambda_t(t - \Delta t)\Big]\Delta t + \mathcal{O}\left([\Delta t]^2\right). \tag{4.14}$$

With the probability balance, Eq. 4.12, we may rearrange by subtracting by $P_n(t-\Delta t)$ and dividing by Δt to find:

$$\begin{aligned}\frac{P_n(t)-P_n(t-\Delta t)}{\Delta t} = &-\Big[S(t-\Delta t)+n\lambda_t(t-\Delta t)-\mathcal{O}\left(\Delta t\right)\Big]P_n(t-\Delta t)\\ &+(n+1)\Big[\lambda_c(t-\Delta t)+\lambda_\ell(t-\Delta t)\Big]P_{n+1}(t-\Delta t)\\ &+S(t-\Delta t)\sum_{\nu=0}^{\nu_m^S}q_\nu^S P_{n-\nu}(t-\Delta t)\\ &+\lambda_f(t-\Delta t)\sum_{\nu=0}^{\nu_m^f}q_\nu^f(n+1-\nu)P_{n+1-\nu}(t-\Delta t).\end{aligned} \tag{4.15}$$

If we next take the limit as $\Delta t \to 0$, the LHS of Eq. 4.15 is simply the limit definition of a derivative with respect to t. We then arrive at a linear first-order ordinary differential-difference (DDE) equation satisfied by $P_n(t)$:

$$\begin{aligned}\frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = &-\Big[S(t)+n\lambda_t(t)\Big]P_n(t)+(n+1)\Big[\lambda_c(t)+\lambda_\ell(t)\Big]P_{n+1}(t)\\ &+S(t)\sum_{\nu=0}^{\nu_m^S}q_\nu^S P_{n-\nu}(t)+\lambda_f(t)\sum_{\nu=0}^{\nu_m^f}q_\nu^f(n+1-\nu)P_{n+1-\nu}(t).\end{aligned} \tag{4.16}$$

with $n=0,1,2,\ldots$. The initial condition is given by:

$$P_n(t=t_o)=\delta_{n,m} \tag{4.17}$$

where m is the initial number of neutrons within the system and $\delta_{i,j}$ is the Kronecker delta function. Equation 4.16 is the Forward Master Equation (FME) for the model defined in Sec. 4.1 where we have allowed for capture and leakage events and arbitrary neutron number emission from SEs and IFEs. The FME describes the temporal change in the population distribution due to the effects present on the RHS of the equation. The first term on the RHS is negative because those are loss mechanisms that cause the population to leave state n and therefore cause the change over time (derivative) of state n to decrease. The other terms on the RHS are "sources" that contribute to state n from other states and therefore cause the derivative of state n to increase.

The system of equations for $n=0,1,2,\ldots,\infty$ is open, meaning that each equation is dependent on the solution to the next highest DDE, due to the P_{n+1} term (note that there is a P_{n+1} also from the IF sum when $\nu=0$). This is one of the features that drastically complicates solving this equation because it requires solving the system of equations for all n simultaneously (remember there are an infinite number of equations). Alternatively, and what has been done numerically in practice [19], we may truncate the distribution at some large $n=N$ by assuming $P_{N+1}\approx 0$ which closes the system, but this is only accurate for systems in which the neutron population is not growing (i.e., subcritical systems). As before, we vie to solve this open set of equations by converting it to a single PDE satisfied by the probability generating function. We perform this transformation next.

4.2.2 Equation for the Probability Generating Function

In this section, we employ a transformation method on the Master equation which effectively consolidates the infinite number of differential-difference equations into a single equation for the transform

function. The transform takes the form of the probability generating function (PGF). The PGF is an attractive candidate because it is effectively a power series representation of the PDF, which has a well-developed theory established for non-negative coefficients. If X is a discrete random variable taking on values in the non-negative integers, i.e. $\{X \in \mathbb{Z}_{x\geq 0}\}$, then the PGF of X is defined as

$$G(z) = \mathrm{E}\left(z^X\right) = \sum_{x=0}^{\infty} z^x p_x, \tag{4.18}$$

where $\mathrm{E}(\cdot)$ is the expectation operator, p_x is a probability distribution function of X and z is the continuous transform variable. The PGF power series has absolute convergence for all complex numbers z with $|z| \leq 1$, but we will further restrict $\{z \in \mathbb{R}|0 \leq z \leq 1\}$. We mention the relation between G and the expectation operator because we will be using G to derive equations for the moments of the distribution later.

If we specifically define the PGF for the FME, Eq. 4.16, as

$$G(z,t) = \sum_{n=0}^{\infty} z^n P_n(t), \tag{4.19}$$

with the z-derivative given by:

$$\frac{\partial G(z,t)}{\partial z} = \sum_{n=0}^{\infty} n z^{n-1} P_n(t). \tag{4.20}$$

We may multiply Eq. 4.16 by z^n and sum over all n to find

$$\begin{aligned}\sum_{n=0}^{\infty} z^n \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} = & -S(t)\sum_{n=0}^{\infty} z^n P_n(t) - \lambda_t(t)\sum_{n=0}^{\infty} n z^n P_n(t) + (\lambda_c(t)+\lambda_\ell(t))\sum_{n=0}^{\infty}(n+1)z^n P_{n+1}(t) \\ & + S(t)\sum_{n=0}^{\infty} z^n \sum_{\nu=0}^{\nu_m^S} q_\nu^S P_{n-\nu}(t) + \lambda_f(t)\sum_{n=0}^{\infty} z^n \sum_{\nu=0}^{\nu_m^f} q_\nu^f (n-\nu+1) P_{n-\nu+1}(t).\end{aligned} \tag{4.21}$$

We next simplify Eq. 4.21 term-by-term to find an equation for the PGF. It is clear that the left-hand side of Eq. 4.21 may be treated as

$$\begin{aligned}\sum_{n=0}^{\infty} z^n \frac{\mathrm{d}P_n(t)}{\mathrm{d}t} &= \frac{\partial}{\partial t}\sum_{n=0}^{\infty} z^n P_n(t) \\ &= \frac{\partial G(z,t)}{\partial t},\end{aligned} \tag{4.22}$$

and in a similar fashion, the first term on the right-hand side is simply

$$-S\sum_{n=0}^{\infty} z^n P_n(t) = -SG(z,t). \tag{4.23}$$

The next term may be put into terms of G by recalling Eq. 4.20 and multiplying by $z^{-1}z$:

$$\begin{aligned} -\lambda_t \sum_{n=0}^{\infty} n z^n P_n(t) &= -\lambda_t \frac{z}{z} \sum_{n=0}^{\infty} n z^n P_n(t) \\ &= -\lambda_t z \sum_{n=0}^{\infty} n z^{n-1} P_n(t) \\ &= -\lambda_t z \frac{\partial G}{\partial z}. \end{aligned} \tag{4.24}$$

The capture and leakage term is treated by defining a new index $m = n + 1$. Then $n = m - 1$ and the index sum goes from 1 to ∞, however, since the $m = 0$ term will be non-contributing (will be null), we may include it in the summation. Thus, we find

$$\begin{aligned} (\lambda_c + \lambda_\ell) \sum_{n=0}^{\infty} (n+1) z^n P_{n+1}(t) &= (\lambda_c + \lambda_\ell) \sum_{m=0}^{\infty} m z^{m-1} P_m(t) \\ &= (\lambda_c + \lambda_\ell) \frac{\partial G}{\partial z}. \end{aligned} \tag{4.25}$$

We handle the source term by defining an index $m = n - \nu$, then $n = m + \nu$, giving $z^n = z^m z^\nu$, and we find:

$$\begin{aligned} S \sum_{n=0}^{\infty} z^n \sum_{\nu=0}^{\nu_m^S} q_\nu^S P_{n-\nu}(t) &= S \sum_{m=0}^{\infty} z^m z^\nu \sum_{\nu=0}^{\nu_m^S} q_\nu^S P_m(t) \\ &= S \left(\sum_{\nu=0}^{\nu_m^S} z^\nu q_\nu^S \right) \sum_{m=0}^{\infty} z^m P_m(t) \\ &= S g_{_S}(z) G(z,t), \end{aligned} \tag{4.26}$$

where, in going from the first to the second line, we factored out the sum over ν as it is not dependent on m and we recognize that $P_{m<0}(t) = 0$ and we have defined the PGF for the source multiplicity distribution as:

$$g_{_S}(z) = \sum_{\nu=0}^{\nu_m^S} z^\nu q_\nu^S. \tag{4.27}$$

Finally, we may simplify the induced fission term by defining an index $m = n - \nu + 1$, then $z^n = z^{m-1} z^\nu$, and we find

$$\begin{aligned} \lambda_f \sum_{n=0}^{\infty} z^n \sum_{\nu=0}^{\nu_m^f} q_\nu^f (n - \nu + 1) P_{n-\nu+1}(t) &= \lambda_f \left(\sum_{\nu=0}^{\nu_m^f} z^\nu q_\nu^f \right) \sum_{m=0}^{\infty} m z^{m-1} P_m(t) \\ &= \lambda_f g_{_f}(z) \frac{\partial G}{\partial z}, \end{aligned} \tag{4.28}$$

where $g_{_f}(z)$ is the PGF for the induced fission multiplicity distribution

$$g_{_f}(z) = \sum_{\nu=0}^{\nu_m^f} z^\nu q_\nu^f. \tag{4.29}$$

Assembling the identities Eqs. 4.22 - 4.29, we arrive at a PDE satisfied by the PGF:

$$\frac{\partial G(z,t)}{\partial t} = \Big[-\lambda_t(t)z + \lambda_c(t) + \lambda_\ell(t) + \lambda_f(t)g_{_f}(z)\Big]\frac{\partial G(z,t)}{\partial z} + S(t)\big[g_{_S}(z) - 1\big]G(z,t). \tag{4.30}$$

We may determine the initial condition of Eq. 4.30 by applying the PGF to Eq. 4.17 to find

$$G(z,0) = z^m, \tag{4.31}$$

where m is the initial neutron population.

Equation 4.30 is a linear hyperbolic PDE of the forward PGF, which may be solved using the Method of Characteristics under certain conditions. As expected, this PGF PDE is substantially more complicated than the PGF PDE from the previous chapter, Eq. 3.21, due to the additional physics we have included. It is easy to recover Eq. 3.21 by simply removing capture and leakage and by setting $q_\nu^f = \delta_{\nu,2}$ (i.e., 2 and only 2 neutrons per fission) and $q_\nu^S = \delta_{\nu,1}$ (i.e., singlet-emitting source). The newest features include the PGFs for the multiplicity distributions, $g_x(z)$, whose arrival should come as no surprise when we realize that they are simply the transforms of the multiplicative processes for SEs and IFEs. Additionally, one should keep in mind that $g_x(z)$ are essentially ν_m^x-order polynomials in z- this will become important in the next section.

4.2.3 Solutions to the PGF PDE

In this section, we seek analytical solutions to the PGF PDE, Eq. 4.30, restated here:

$$\frac{\partial G(z,t)}{\partial t} = \; g(z,t)\frac{\partial G(z,t)}{\partial z} + S\big[g_{_S}(z) - 1\big]G(z,t),$$

where we have defined the coefficient of the $\partial G/\,\partial z$ term to simplify the following analysis:

$$g(z,t) = \Big[-\lambda_t(t)z + \lambda_c(t) + \lambda_\ell(t) + \lambda_f(t)g_{_f}(z)\Big]. \tag{4.32}$$

In its current general form, Eq. 4.30 does not have a solution in known mathematical functions, but we will steadfastly proceed by recognizing that we may attempt to find solutions using the Method of Characteristics. This is done by comparing Eq. 4.30 with the total derivative of G with respect to time,

$$\frac{\mathrm{d}G}{\mathrm{d}t} = \frac{\partial G}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t} + \frac{\partial G}{\partial t}. \tag{4.33}$$

By inspection, the system of characteristic equations is obtained:

$$\frac{\mathrm{d}z(t)}{\mathrm{d}t} = -g(z(t)) \tag{4.34a}$$

$$\frac{\mathrm{d}G(z(t),t)}{\mathrm{d}t} = S(t)\big[g_{_S}\big(z(t)\big) - 1\big]G(z(t),t). \tag{4.34b}$$

Equation 4.34b is an elementary first-order differential equation that is solved by separation of variables followed by integration over the time domain to yield

$$G(z(t),t) = [z(t_o)]^m \exp\left\{\int_{t_o}^{t} \mathrm{d}t' S(t')\big[g_{_S}\big(z(t')\big) - 1\big]\right\}, \tag{4.35}$$

where we are reminded that $g_{_S}(z(t))$, defined by Eq. 4.27, is an ν_m^S-order polynomial in z. Depending on the form of $z(t)$, obtained by solving Eq. 4.34a, this may prove to be an incalculable integral in and of itself. With that said, we see that Eq. 4.34a takes the integral form:

$$\int_{z(t_o)}^{z(t)} \mathrm{d}z' \frac{1}{g(z')} = \int_{z(t_o)}^{z(t)} \mathrm{d}z' \frac{1}{-\lambda_t z' + \lambda_c + \lambda_\ell + \lambda_f g_{_f}(z')} = -(t - t_o). \tag{4.36}$$

Recalling Eq. 4.29, the definition of $g_f(z(t))$, as being an ν_m^f-order polynomial in z, this integral is not solvable for polynomials greater than order 3, prompting us to explore several solution paths in the remainder of this section.

There are effectively two ways of solving Eq. 4.30 by means of making a mathematical approximation to the equation itself or by restricting the physics of the problem in some way. Both of these approaches vie to lessen the complexity of the characteristic equation, Eq. 4.34a, by lowering the variable coefficient power to order two (recall this provided the Riccati/Bernoulli ODE, Eq. 3.24a, for the BFM). We will only consider the mathematical approximation, namely the Quadratic Approximation, and we have already considered the physics approximation, the Binary Fission Model, in the previous chapter. We could apply the BFM to this problem, but we leave that as an exercise, and we proceed by apply the Quadratic Approximation.

4.2.4 The Quadratic Approximation

We wish to solve Eq. 4.34a by approximating the form of $g(z(t))$, defined by Eq. 4.32. This is accomplished by expanding g in a Taylor series about $z = 1$ and retaining only up to the second order terms; for this reason, this methodology is commonly referred to as the Quadratic Approximation (QA). Originally performed by Bell in obtaining the neutron number distribution for large neutron populations [9], and later employed by Prinja and Souto [16] to extract the discrete number distribution- both for the FME- we henceforth follow the same procedure as Prinja and Souto.

In advancing, we recall the definition of the total reaction rate, $\lambda_t = 1/\tau$ from Eq. 1.10c, and the supplementary reaction rates as $\lambda_x = p_x/\tau$, Eq. 4.32 may be rewritten as:

$$g(z) = \frac{1}{\tau}\left[-z + p_c + p_\ell + p_f \sum_{\nu=0}^{\nu_m^f} z^\nu q_\nu^f\right].$$

If we now expand $-z + p_f \sum_\nu z^\nu q_\nu^f$ in a Taylor series about $z = 1$, we find

$$\begin{aligned}
-z + p_f \sum_\nu z^\nu q_\nu^f = &\left[-z + p_f \sum_\nu z^\nu q_\nu^f\right]\Bigg|_{z=1} + \left[-1 + p_f \sum_\nu \nu z^{\nu-1} q_\nu^f\right]\Bigg|_{z=1} (z-1) \\
&+ \frac{p_f}{2!} \sum_\nu \nu(\nu-1) z^{\nu-2} q_\nu^f \Bigg|_{z=1} (z-1)^2 + \cdots \\
&= (-1 + p_f) + (-1 + p_f \overline{\nu})(z-1) + \frac{p_f (z-1)^2}{2!} \sum_\nu \nu(\nu-1) q_\nu^f \\
&+ \frac{p_f (z-1)^3}{3!} \sum_\nu \nu(\nu-1)(\nu-2) q_\nu^f + \cdots
\end{aligned}$$

Noting the identities $k = p_f \overline{\nu}$ (from Eq. 1.7), $\nu(\nu-1)\cdots(\nu-m+1) = \nu!/(\nu-m)!$, and $1 = p_f + p_c + p_\ell$,

we may write

$$g(z) = \frac{1}{\tau}\left[(k-1)(z-1) + p_f \sum_{m=2}^{\infty}\sum_{\nu=0}^{\nu_m^f} \frac{\nu!}{(\nu-m)!} q_\nu^f \frac{(z-1)^m}{m!}\right].$$

Further, by recognizing that for $m > \nu_m^f$ the binomial coefficient in the above equation is zero, and similarly for $\nu < m$, we may rewrite g as

$$\begin{aligned} g(z) &= \frac{1}{\tau}\left[(k-1)(z-1) + p_f \sum_{m=2}^{\nu_m^f}\sum_{\nu=m}^{\nu_m^f} \frac{\nu!}{(\nu-m)!} q_\nu^f \frac{(z-1)^m}{m!}\right] \\ &= \frac{1}{\tau}\left[(k-1)(z-1) + p_f \sum_{m=2}^{\nu_m^f} \chi_m \frac{(z-1)^m}{m!}\right] \end{aligned} \tag{4.37}$$

where χ_m is defined as

$$\chi_m = \sum_{\nu=m}^{\nu_m^f} \frac{\nu!}{(\nu-m)!} q_\nu^f. \tag{4.38}$$

We have yet to make an approximation to g, but this is done now by truncating the sum in Eq. 4.37 at $\nu_m^f = 2$, giving us a quadratic polynomial in z:

$$g(z) \approx \frac{1}{\tau}\left[(k-1)(z-1) + p_f \chi_2 \frac{(z-1)^2}{2}\right]. \tag{4.39}$$

This is known as the Quadratic Approximation, and it allows us to solve the characteristic equation for $z(t)$. Although we used the symbol ν_m^f in the above when truncating, this does not mean we are removing the effects of the higher neutron multiplets from our analysis. This is seen by recognizing these higher emission probabilities may still be used when calculating χ_2 in Eq. 4.38. This is crucial because it allows us to consider the full multiplicity distribution and the approximation is that the second factorial moment, χ_2, sufficiently represents the induced fission propagation process. We note the identities: $\chi_0 = 1$ is the zeroth moment of the multiplicity distribution (the normalization) and $\chi_1 = \overline{\nu}$ is the first moment, the mean. Also, we note that τ, p_f, and k may be time-dependent, but no loss of generality has been had up to this point.

4.2.5 Solution via the QA

With the QA in-hand, we proceed by solving the approximated form of Eq. 4.34a, by first introducing the substitution

$$u(t) = z(t) - 1, \tag{4.40}$$

along with the two variables:

$$\alpha(t) = \frac{k(t)-1}{\tau(t)}, \tag{4.41a}$$

$$\chi_2'(t) = \frac{p_f(t)\chi_2}{\tau(t)}, \tag{4.41b}$$

to then find Eq. 4.34a as:

$$\frac{\mathrm{d}u(t)}{\mathrm{d}t} = -g(u(t),t) = -\alpha(t)u(t) - \frac{\chi_2'(t)}{2}\big[u(t)\big]^2. \tag{4.42}$$

The nonlinear ODE of the characteristic curve in the QA is of the Riccati-type (more precisely it is a Bernoulli equation because it is homogeneous). Any Bernoulli equation of nonlinear order k can be reduced to a linear ODE by making the substitution $y = u^{1-k}$. Setting $k = 2$, we arrive at a linear equation in $y = 1/u$:

$$\frac{\mathrm{d}y}{\mathrm{d}t} = \alpha(t)y(t) + \frac{\chi_2'(t)}{2},$$

which is solved using the integrating factor technique over the time domain $t' \in [t_o, t]$. An equation for $u(t)$ is ultimately acquired

$$\begin{aligned}\frac{1}{u(t)} &= \frac{1}{u(t_o)} \exp\left\{\int_{t_o}^{t} \mathrm{d}t' \alpha(t')\right\} + \int_{t_o}^{t} \mathrm{d}t' \frac{\chi_2'(t')}{2} \exp\left\{\int_{t'}^{t} \mathrm{d}t'' \alpha(t'')\right\} \\ &= \frac{1}{u(t_o)} a(t) + b(t) \end{aligned} \tag{4.43}$$

where we have defined

$$a(t) = \exp\left\{\int_{t_o}^{t} \mathrm{d}t' \alpha(t')\right\} \tag{4.44a}$$

$$b(t) = \int_{t_o}^{t} \mathrm{d}t' \frac{\chi_2'(t')}{2} \exp\left\{\int_{t'}^{t} \mathrm{d}t'' \alpha(t'')\right\}. \tag{4.44b}$$

We next insert Eq. 4.43 into the expression for G, Eq. 4.35, in order to solve the PGF equation, Eq. 4.30, for which the final result will depend on the initial condition (i.e., the initial neutron population). In terms of the substituted variable, u, the G characteristic equation solution becomes

$$G(u(t), t) = [u(t_o) + 1]^m \exp\left\{\int_{t_o}^{t} \mathrm{d}t' S(t') \big[g_s\big(u(t') + 1\big) - 1\big]\right\}. \tag{4.45}$$

We proceed by addressing the two primary cases that are examined in practice: the case of a single initial neutron without a source present (which we have been referring to as the single chain case), and the case of zero initial neutrons in the presence of a source.

Single Chain Case

For the case of a single initial neutron without a source present, we simply set $S = 0\ s^{-1}$ and we set $m = 1$ in Eq. 4.45. This tells us that $\mathrm{d}G/\,\mathrm{d}t = 0$ (from Eq. 4.34b), and the PGF is constant along the characteristic curve and is simply equal to the initial condition, i.e.,

$$G(u(t), t) = G(u(t_o), t_o) = 1 + u(t_o). \tag{4.46}$$

Solving Eq. 4.43 for $u(t_o) = a/(1/u - b)$ and recovering explicit z-dependence yields

$$G(z(t), t) = 1 + \frac{a(t)}{\frac{1}{z-1} - b(t)}. \tag{4.47}$$

Equation 4.47 is in the ideal form, and our next task will be to invert G to determine the single chain neutron number distribution, discussed in Sec. 4.2.6. This is the solution obtained originally by Bell [9] and later by Prinja & Souto [16].

Source Case

The case of a source with no initial neutrons is, unsurprisingly, more involved than the single chain case due to the retention of the exponential functional form of G. In reference to Eq. 4.45, we set $m = 0$ to find

$$G(u(t), t) = \exp\left\{\int_{t_o}^{t} \mathrm{d}t' S(t') \left[-1 + \sum_{\nu=0}^{\nu_m^S} q_\nu^S \left(1 + \left[\frac{a(t')}{u(t_o)} + b(t')\right]^{-1}\right)^{\nu}\right]\right\} \tag{4.48}$$

and we see that the source multiplicity distribution PGF introduces complications due to the ν_m^S-order power of the argument, $1 + u(t')$. For this reason, the integral is not easily computed and we therefore make the assumption that the source is:

- constant in time,
- and singlet emitting, i.e. $q_\nu^S = \delta_{\nu,1}$.

After rearranging, this assumption dramatically simplifies Eq. 4.48:

$$G(u(t), t) = \exp\left\{S \int_{t_o}^{t} \mathrm{d}t' \frac{u(t_o)/a(t')}{1 + u(t_o)\frac{b(t)}{a(t)}}\right\}. \tag{4.49}$$

At this time, we need to further assume χ_2' is time-independent such that $b(t)$ can be simplified to provide

$$G(u(t), t) = \exp\left\{S u(t_o) \int_{t_o}^{t} \mathrm{d}t' \frac{j(t')}{1 + \frac{u(t_o)\chi_2'}{2} \int_{t_o}^{t'} \mathrm{d}t'' j(t'')}\right\}. \tag{4.50}$$

where we have made the substitution $j(t') = 1/a(t') = \exp\{\int_{t'}^{t_o} \mathrm{d}t'' \alpha(t'')\}$. If we further define $J(t') = \int_{t_o}^{t'} \mathrm{d}t'' j(t'')$, then $\mathrm{d}J/\,\mathrm{d}t' = j(t')$ and the integral may be further simplified and ultimately solved:

$$\int_0^{J(t')} \mathrm{d}J \frac{1}{1 + \frac{u(t_o)\chi_2'}{2} J} = \frac{2}{u(t_o)\chi_2'} \ln\left[1 + \frac{u(t_o)\chi_2'}{2} \int_{t_o}^{t} \mathrm{d}t' \exp\left\{\int_{t'}^{t_o} \mathrm{d}t'' \alpha(t'')\right\}\right].$$

This gives us the solution

$$G(u(t), t) = \left[1 + \frac{\chi_2'}{2}\left(\frac{a(t)u}{1 - ub(t)}\right) \int_{t_o}^{t} \mathrm{d}t' \exp\left\{\int_{t'}^{t_o} \mathrm{d}t'' \alpha(t'')\right\}\right]^{\eta}, \tag{4.51}$$

where we have eliminated $u(t_o)$ and we have introduced the parameter, often called Bell's parameter,

$$\eta = \frac{2S}{\chi_2'}. \tag{4.52}$$

We may further simplify the Eq. 4.51 by recalling the definition of $a(t)$, pushing it into the integral, recognizing the relation to $b(t)$, and converting back to terms of z to find

$$G(z(t), t) = \left[1 - \big(z - 1\big)b(t)\right]^{-\eta}. \tag{4.53}$$

As a reminder, Eq. 4.53 was obtained for the specific case of a singlet emitting source, where we further assumed the source, S, and χ_2' to be time-independent (keep in mind that χ_2' is constant when calculating $b(t)$). It was shown that we did not need to make an assumption on the form of $\alpha(t)$, allowing us to maintain a general time-dependence on the system criticality. Equation 4.53 is in the ideal form to invert G to recover the neutron number distribution in the presence of a source, $P_n(t)$, to be discussed in next.

4.2.6 Inversion of the PGF

In this section, we show how to invert the ascertained expressions for the forward PGFs to obtain the neutron number distribution. The process is the same as before, but we show it now for completeness. In essence, we vie to manipulate the PGF solutions to put them into a form that allows us to expand it into a Taylor series about $z = 0$- from which, we will extract the number distributions by inspection.

Single Chain

In the application of the QA for the single chain case, we arrived at an approximate solution to Eq. 4.30 by truncating the Taylor series expansion of the characteristic equation for z at second order, given by Eq. 4.47, restated and rearranged here:

$$\begin{aligned} G(z,t) &= 1 + \frac{(z-1)a(t)}{1-(z-1)b(t)} \\ &= 1 + \frac{(z-1)a(t)}{1+b(t)} \left[1 - \frac{b(t)}{1+b(t)} z\right]^{-1}. \end{aligned} \tag{4.54}$$

Since $0 \leq b/(1+b) \leq 1$ and $0 \leq z \leq 1$, then $0 \leq bz/(1+b) \leq 1$, and we may therefore expand the bracketed term in a Taylor series about $z = 0$ (which, by the way, is also the Binomial Theorem in this instance); doing so provides

$$G(z,t) = 1 + \frac{(z-1)a(t)}{1+b(t)} \sum_{n=0}^{\infty} \left[\frac{b(t)}{1+b(t)}\right]^n z^n. \tag{4.55}$$

Next, we absorb the $(z-1)$ factor into the summation,

$$G(z,t) = 1 + \frac{a(t)}{1+b(t)} \left[\sum_{n=0}^{\infty} \left[\frac{b(t)}{1+b(t)}\right]^n z^{n+1} - \sum_{n=0}^{\infty} \left[\frac{b(t)}{1+b(t)}\right]^n z^n\right],$$

and by shifting the index of the first summation, $m = n+1$, we find

$$G(z,t) = 1 + \frac{a(t)}{1+b(t)} \left[\sum_{m=1}^{\infty} \left[\frac{b(t)}{1+b(t)}\right]^{m-1} z^m - \sum_{n=0}^{\infty} \left[\frac{b(t)}{1+b(t)}\right]^n z^n\right].$$

By isolating the $n = 0$ term in the second sum, the summation may be combined and we arrive at the ultimate desired form of G:

$$G(z,t) = 1 - \frac{a(t)}{1+b(t)} + \frac{a(t)}{\left[1+b(t)\right]^2} \sum_{n=1}^{\infty} \left[\frac{b(t)}{1+b(t)}\right]^{n-1} z^n. \tag{4.56}$$

Comparing Eq. 4.56 to the original definition of the generating function,

$$G(z,t) = \sum_{n=0}^{\infty} P_n(t) z^n,$$

we see that the extinction probability is already isolated and the remainder of the distribution may be inferred accordingly:

$$P_0(t) = 1 - \frac{a(t)}{1+b(t)} \tag{4.57a}$$

$$P_n(t) = \frac{a(t)}{\big[1+b(t)\big]^2}\left[\frac{b(t)}{1+b(t)}\right]^{n-1}, \qquad n = 1,2,3,\ldots. \tag{4.57b}$$

Equations 4.57a and 4.57b constitute the discrete neutron number distribution in the Quadratic Approximation. First obtained by Prinja and Souto [16], this PDF is a natural generalization to Bell's single chain distribution [9]. For this reason, we refer to Eq. 4.57 as the Prinja-Souto distribution for the single neutron chain number distribution.

In the Presence of a Source

We are now interested in inverting the forward PGF solution in the presence of a source, given by Eq. 4.53. The process is wholly the same as for the single chain case, but the resulting distribution is categorically different, as will be seen. Equation 4.53 is already in the ideal format after a simple factorization,

$$\begin{aligned} G(z,t) &= \Big[1 - \big(z-1\big)b(t)\Big]^{-\eta} \\ &= \frac{1}{\big(1+b(t)\big)^{\eta}}\left[1 - \frac{b(t)}{1+b(t)}z\right]^{-\eta}, \end{aligned} \tag{4.58}$$

we may expand the bracketed term into a Taylor series about $z = 0$. In doing so, Eq. 4.58 becomes

$$G(z,t) = \frac{1}{\big(1+b(t)\big)^{\eta}} \sum_{n=0}^{\infty} \frac{\eta(\eta+1)\cdots(\eta+n-1)}{m!}\left[\frac{b(t)}{1+b(t)}\right]^n z^n. \tag{4.59}$$

The rising factorial of η may be written in terms of the Gamma function facilitated by the identity:

$$\eta(\eta+1)\cdots(\eta+n-1) = \frac{\Gamma(\eta+n)}{\Gamma(\eta)}. \tag{4.60}$$

As before, if we then compare Eq. 4.59 to the definition of the PGF, $G(z,t) = \sum_{n=0}^{\infty} P_n(t) z^n$, we may readily extract the number distribution in the presence of a source:

$$\begin{aligned} P_n(t) &= \frac{1}{\big(1+b(t)\big)^{\eta}}\left[\frac{\Gamma(\eta+n)}{n!\,\Gamma(\eta)}\right]\cdot\left[\frac{b(t)}{1+b(t)}\right]^n, \qquad n = 0,1,2,\ldots \\ &= \frac{\eta+n-1}{n}\cdot\frac{b(t)}{1+b(t)}P_{n-1}(t) \;\text{ with } P_0(t) = (1+b(t))^{-\eta}, \end{aligned} \tag{4.61}$$

where we have written P_n recursively to remove computation of the gamma function, which has issues for large n. Equation 4.61 is the discrete neutron number PDF in the QA, first obtained by Prinja and Souto [16]. As with the previous section for the single chain distribution, this PDF is a generalization of Bell's distribution [9] in the presence of a source. Equation 4.61 is referred to as the Prinja-Souto distribution in the presence of a constant singlet-emitting neutron source.

4.3 Backward Formulation

In this section, we consider the other primary formulation method for obtaining the neutron number probability distribution function, in lumped phase space, referred to as the Backward Master Equation Formulation [18]. The probability balance is conducted over the *first* collision interval in the backward formulation, as opposed to the forward formulation in which the balance is constructed over the *last* collision interval. In constructing the balance in the forward setting, we determined what states are connected to the state n and by what mechanisms will those states lead to state n (i.e., capture, leakage, fission) over some short time interval. In the backward setting, we assume a *single* neutron appears at some time and the balance is then conducted to account for all events the neutron will undergo in a short time interval and then from those events, what are the connected probabilistic states that will then lead to state n.

As a final supplemental contrast, in the forward approach there is no single initial state to produce the balance, but the backward approach requires such. We then assert that a single neutron is injected at the earlier time and conduct our balance over the first collision interval. With the initial state being known, we are therefore unable to incorporate a randomly emitting source into the balance as the solution loses uniqueness. Therefore, we will then need to perform a separate balance that accounts for random source emissions. For this reason, we have separated this section into a single neutron chain formulation followed by the auxiliary balance for the inclusion of a source.

4.3.1 Probability Balance & Master Equation

We define the time intervals of interest for the single chain and source probability balances:

$$I_b = [t_o, t_o + \Delta t_o] \tag{4.62a}$$

$$I_b^c = [t_o + \Delta t_o, t] \tag{4.62b}$$

where we see that the entire time interval, from introduction of the source at t_o to observation of the system at t, is given by $I_b + I_b^c$. Also, we use the superscript c to denote the complement.

Single Chain

As was stated above, we first construct a probability balance for a single initial neutron introduced into the system at some time t_o and sum all mutually exclusive events the neutron may experience which will then lead to n neutrons within the system at some later time t, stated in words as:

$$P_n(t|t_o) = \begin{array}{l}\text{the probability of there existing } n \text{ neutrons within the system at time } t \text{ due} \\ \quad \text{to the introduction of a single neutron at an earlier time } t_o.\end{array} \tag{4.63}$$

For the single initial neutron, the list of mutually exclusive events that occur in the first collision interval, I_b, are:

1. the neutron does not collide with a nucleus composing the medium,
2. the neutron does collide, which results in two possible interactions:
   (a) is captured and the chain ends,
   (b) is absorbed and induces a fission, producing ν neutrons with probability q_ν^f,
3. or the neutron leaks from the system and the chain ends.

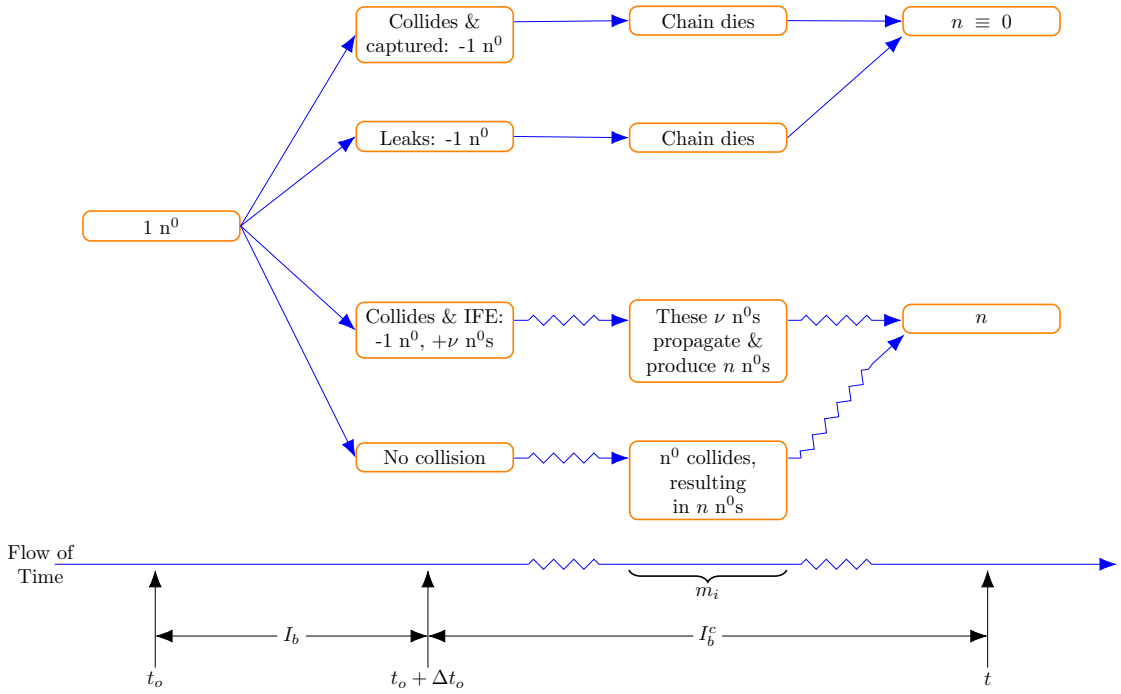


Figure 4.2: Mutually exclusive events that a single neutron may experience in I_b followed by the possible paths in the remaining time I_b^c that will result in n neutrons at time t.

Let us again proceed with a cautionary note. We assume Δt_o is sufficiently small such that if a collision occurs the resulting effects will not have time to interact with the system. Also, although Δt_o is very small, the difference in time between $t_o + \Delta t_o$ and t (i.e. I_b^c) is arbitrarily large. Thus, there could be additional events that may occur in the remaining time I_b^c and we will need to include that possibility in our probability balance. To further illustrate this, Fig. 4.2 shows the events and how they may occur over the total time interval, where we note that the zig-zigs mean an arbitrary passage of time and IFE stands for induced fission event. In this figure, we see the list of events that may occur in I_b, followed by a passage of time in I_b^c where the neutron chain propagates ultimately resulting in n neutrons at t. For the case of a neutron being captured or leaking, the chain immediately ends and we have therefore not included 'zig-zags' on the state transitions as this effect instantaneously takes place and the only contributing state is the empty state, $n \equiv 0$. For the case of an IFE occurring in I_b, there will be an emission of ν neutrons with probability q_ν^f and those ν neutrons will propagate and each branch will produce a population $n_1, n_2, \ldots, n_\nu$ such that $n_1 + n_2 + \cdots + n_\nu = n$ in order for that probability set to contribute to $P_n(t|t_o)$. Also, the neutron may not collide or leak in I_b, and it will therefore continue to travel through the system during I_b^c whence it will eventually collide or leak, resulting in n neutrons at time t.

The probability balance in words is then:

$$
\begin{aligned}
P_n(t|t_o) = &\begin{pmatrix}\text{Probability the initial n}^0\text{ does}\\ \text{not collide or leak in } I_b\end{pmatrix} \times \begin{pmatrix}\text{Probability the initial n}^0\text{ interacts}\\ \text{in } I_b^c,\text{ resulting in } n \text{ neutrons at } t\end{pmatrix} \\
&+ \left[\begin{pmatrix}\text{Probability initial n}^0\\ \text{is captured in } I_b\end{pmatrix} + \begin{pmatrix}\text{Probability initial n}^0\\ \text{leaks in } I_b\end{pmatrix}\right] \times \begin{pmatrix}\text{Probability of being in}\\ \text{state } n \equiv 0 \text{ at time } t\end{pmatrix} \\
&+ \begin{pmatrix}\text{Probability initial n}^0\\ \text{causes an IFE in } I_b\end{pmatrix} \times \Bigg[\begin{pmatrix}\text{Probability of 0 n}^0\text{s}\\ \text{being emitted}\end{pmatrix} \times \begin{pmatrix}\text{Probability of being in}\\ \text{state } n \equiv 0 \text{ at time } t\end{pmatrix} \\
&\qquad + \begin{pmatrix}\text{Probability of 1 n}^0\\ \text{being emitted}\end{pmatrix} \times \begin{pmatrix}\text{Probability of being in state}\\ n \text{ at time } t \text{ due to that 1 n}^0\end{pmatrix} \\
&\qquad + \begin{pmatrix}\text{Probability of 2 n}^0\text{s}\\ \text{being emitted}\end{pmatrix} \times \begin{pmatrix}\text{Probability of being in state}\\ n \text{ at time } t \text{ due to those 2 n}^0\text{s}\end{pmatrix} \\
&\qquad \vdots \\
&\qquad + \begin{pmatrix}\text{Probability of } \nu_m^f \text{ n}^0\text{s}\\ \text{being emitted}\end{pmatrix} \times \begin{pmatrix}\text{Probability of being in state } n\\ \text{at time } t \text{ due to those } \nu_m^f \text{ n}^0\text{s}\end{pmatrix}\Bigg]
\end{aligned}
\tag{4.64}
$$

We can define the probability of a collision occurring in I_b by noting the definition of the total reaction rate as "the probability per neutron per unit time that a collision or leakage will occur," which is written as:

$$
\begin{pmatrix}\text{Probability initial n}^0\\ \text{collides or leaks in } I_b\end{pmatrix} = \lambda_t(t_o)\Delta t_o, \tag{4.65}
$$

where the total reaction rate is taken at the beginning of the time interval I_b and is defined as:

$$
\lambda_t = \lambda_c + \lambda_\ell + \lambda_f. \tag{4.66}
$$

It follows then that the probability of not colliding in I_b is:

$$
\begin{pmatrix}\text{Probability initial n}^0\text{ does}\\ \text{not collide or leak in } I_b\end{pmatrix} = 1 - \lambda_t(t_o)\Delta t_o. \tag{4.67}
$$

Additionally, the probability the initial neutron may be captured, leak, or induce a fission in I_b is given by $\lambda_c(t_o)\Delta t_o$, $\lambda_\ell(t_o)\Delta t_o$, and $\lambda_f(t_o)\Delta t_o$, respectively. In the event that the chain dies in I_b, we know there will be 0 neutrons at time t due to that initial neutron and therefore the probability of there being 0 neutrons at t is certain:

$$
\begin{pmatrix}\text{Probability of being in}\\ \text{state } n \equiv 0 \text{ at time } t\end{pmatrix} = \delta_{n,0}, \tag{4.68}
$$

where $\delta_{n,0}$ is the Kronecker delta. Thus, this term only appears for the equation where $n = 0$, i.e. the LHS of Eq. 4.64 is $P_0(t|t_o)$.

Next, we focus on the multiplication process following an IFE. From the multiplicity distribution, we know "the probability of ν neutrons being emitted" following an IFE from experimental data:

$$
\begin{pmatrix}\text{Probability of } \nu \text{ n}^0\text{s}\\ \text{being emitted}\end{pmatrix} = q_\nu^f, \tag{4.69}
$$

with $\nu = 0, 1, \ldots, \nu_m^f$. We then need to consider the events that follow the emission of the fission neutrons and how they probabilistically propagate in I_b^c. Starting with the emission of a single neutron, we then require that single neutron, emitted at time $t_o + \Delta t_o$, to result in n neutrons at t and thus the connected state probability is $P_n(t|t_o + \Delta t_o)$. For the case of 2 neutrons being emitted from a fission at time $t_o + \Delta t_o$, we suppose one of those neutrons results in n_1 neutrons at time t and the other results in n_2 neutrons at time t such that the sum of those two branches is $n_1 + n_2 = n$. Thus, the connected state is a combination of two states $P_{n_1}(t|t_o + \Delta t_o) \times P_{n_2}(t|t_o + \Delta t_o)$ and, because n_1 and n_2 can be any combination of populations less than or equal to n, we must sum over those possible combinations to find:

$$\begin{pmatrix}\text{Probability those 2 n}^0\text{s produce } n_1 \text{ and} \\ n_2 \text{ n}^0\text{s, such that } n_1 + n_2 = n, \text{ in } I_b^c\end{pmatrix} = \sum_{n_1+n_2=n} P_{n_1}(t|t_o + \Delta t_o) P_{n_2}(t|t_o + \Delta t_o). \tag{4.70}$$

For now, we will keep the summation notation that we have written above, but this sum is really a double sum over all possible combinations of n_1 and n_2 that satisfy the condition $n_1 + n_2 = n$. For ν neutrons being emitted in a fission at time $t_o + \Delta t_o$, we write the following:

$$\begin{pmatrix}\text{Probability the } \nu \text{ n}^0\text{s produce } n_1, n_2, \ldots n_\nu \\ \text{n}^0\text{s, such that } n_1 + n_2 + \cdots + n_\nu = n, \text{ in } I_b^c\end{pmatrix} = \sum_{\substack{n_1+n_2+ \\ \cdots+n_\nu=n}} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o + \Delta t_o), \tag{4.71}$$

where the sum is really a ν-tuple sum where the condition $\sum_{i=1}^{\nu} n_i = n$ is satisfied for a given index value. Finally, the entirety of the second bracketed term of Eq. 4.64 can be written as a sum over all ν from 0 to ν_m^f with that sum being applied to Eq. 4.71, i.e.,

$$\sum_{\nu=0}^{\nu_m^f} q_\nu^f \sum_{n_1+\ldots+n_\nu=n} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o + \Delta t_o).$$

Assembling all of the above, we convert Eq. 4.64 into the Chapman-Kolmogorov equation for the first collision interval probability balance for an initial neutron:

$$\begin{aligned} P_n(t|t_o) = &\Big[1 - \lambda_t(t_o)\Delta t_o\Big] P_n(t|t_o + \Delta t_o) + \Big[\lambda_c(t_o) + \lambda_\ell(t_o)\Big]\Delta t_o \delta_{n,0} \\ &+ \lambda_f(t_o)\Delta t_o \sum_{\nu=0}^{\nu_m^f} q_\nu^f \sum_{n_1+\cdots+n_\nu=n} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o + \Delta t_o). \end{aligned} \tag{4.72}$$

Next, we divide by Δt_o and subtract $P_n(t|t_o + \Delta t_o)$ to find:

$$\begin{aligned} -\frac{P_n(t|t_o + \Delta t_o) - P_n(t|t_o)}{\Delta t_o} = &- \lambda_t(t_o) P_n(t|t_o + \Delta t_o) + \Big[\lambda_c(t_o) + \lambda_\ell(t_o)\Big]\delta_{n,0} \\ &+ \lambda_f(t_o) \sum_{\nu=0}^{\nu_m^f} q_\nu^f \sum_{n_1+\cdots+n_\nu=n} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o + \Delta t_o). \end{aligned} \tag{4.73}$$

On the LHS, we have placed the $P_n(t|t_o + \Delta t_o)$ in front of the $P_n(t|t_o)$ and if we now evaluate the limit as $\Delta t_o \to 0$, the LHS becomes the derivative of $P_n(t|t_o)$ with respect to t_o, and we thus have:

$$-\frac{\partial P_n(t|t_o)}{\partial t_o} = -\lambda_t(t_o) P_n(t|t_o) + \Big[\lambda_c(t_o) + \lambda_\ell(t_o)\Big]\delta_{n,0} + \lambda_f(t_o) \sum_{\nu=0}^{\nu_m^f} q_\nu^f \sum_{n_1+\cdots+n_\nu=n} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o), \tag{4.74}$$

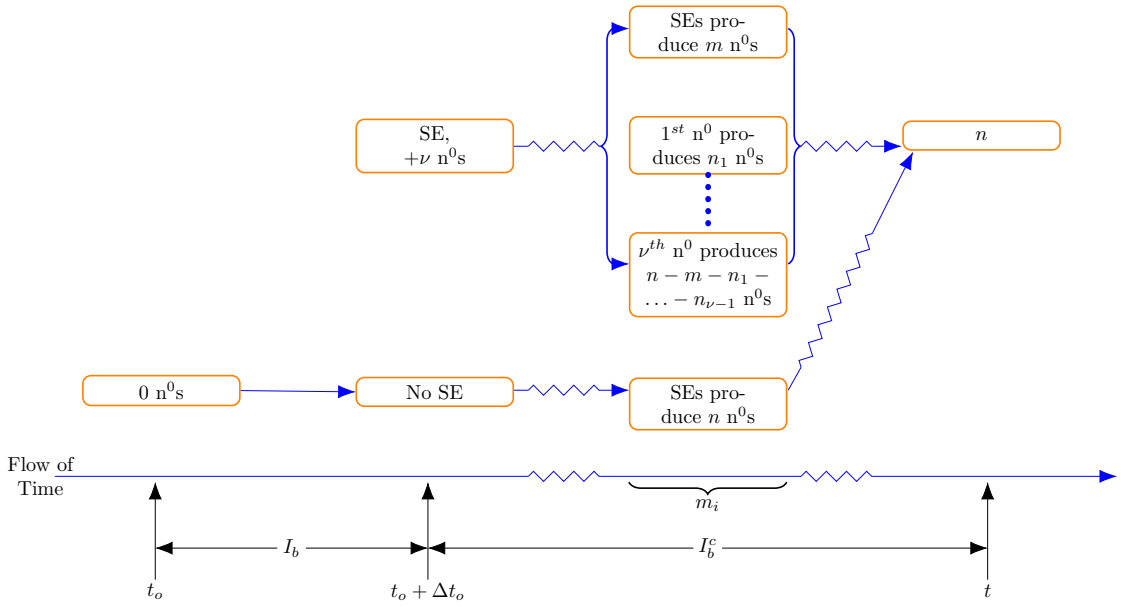


Figure 4.3: Mutually exclusive events that may occur in the backward formulation with a source that emits arbitrary multiplets of neutrons per source event.

with $n = 0, 1, 2, \ldots$. We have obtained the backward master equation for the neutron number distribution due to the introduction of a single neutron at time t_o in a neutron-multiplying system. The 'final' condition is:

$$\lim_{t_o \to t} P_n(t|t_o) = \delta_{n,1} \tag{4.75}$$

where $\delta_{i,j}$ is the Kronecker delta function. This condition tells us that as we bring the neutron injection time t_o up to the time of observation t, the probability of there being one neutron in the system is guaranteed.

A difference between this equation and that of the FME, Eq. 3.13 with $S = 0$, is that the BME is ν_m^f-order nonlinear (due to the products $P_{n_1} P_{n_2} \cdots P_{n_{\nu_m^f}}$). This nonlinearity has appeared because we need to consider all the possible independent probabilistic combinations that will result in n neutrons at t due to the ν_m^f independent chains produced in the IFE in the first collision interval. This is a natural generalization of the BFM model of Chapter 3, Eq. 3.50, which can be obtained by simply setting $\lambda_c = \lambda_\ell = 0$ and $q_\nu^f = \delta_{\nu,2}$.

Source

The probability balance and BME derivation for the source case proceeds by defining the probabilistic quantity of interest:

$$\Theta_n(t|t_o) = \text{the probability of there existing } n \text{ neutrons within the system at time } t \text{ due to the introduction of a source of strength } S \text{ at an earlier time } t_o. \tag{4.76}$$

Let us first consider the events that may take place in the first collision interval I_b, from which we will be able to write down the probability balance in words. The list of mutually exclusive events

that occur in the first collision interval, I_b, are the same as before:

1. No source event occurs
2. A source event occurs, producing ν neutrons.

Note that we assume there are initially zero neutrons within the system and thus no neutron interactions/collisions can occur. Once again, recall Δt_o is sufficiently small such that only one event may occur in Δt_o. We now need to consider the possible pathways stemming from the list above that may lead to the state-space n at time t. In other words, given the two events that may occur in I_b, what consequential events will occur in I_b^c that will lead to n neutrons at t. Using Fig. 4.3, we see that if there is no source event (SE) in I_b, then there must be a collection of source events in I_b^c that lead to n neutrons at t. If there is a SE, then any number from 1 to ν_m^S neutrons are emitted and we therefore must consider that neutron's progeny (i.e., the neutrons produced in the fission chain) resulting in $n_1, n_2, \ldots, n_{\nu_m^S}$ neutrons as well as subsequent SEs resulting in $m = n - n_1 - n_2 - \cdots - n_{\nu_m^S - 1}$ neutrons. Note here that $n = m + n_1 + n_2 + \cdots + n_{\nu_m^S}$, because if it does not then this particular set of events will not contribute to the LHS of Eq. 4.76. We also note that we do not consider the emission of 0 neutrons from a source event as that does not change the state of the system and begs the question, "if a source event does not emit a neutron, is it really a neutron source event?" (of course we would need to consider this event if we were keeping track of photons produced, energy deposited, etc.).

With this, we may define a probability balance in words:

$$\begin{aligned}
\Theta_n(t|t_o) = &\begin{pmatrix} \text{Probability of no SE} \\ \text{occurring in } I_b \end{pmatrix} \times \begin{pmatrix} \text{Probability of subsequent} \\ \text{SEs occurring in } I_b^c, \\ \text{resulting in } n \text{ n}^0\text{s at } t \end{pmatrix} + \begin{pmatrix} \text{Probability of a SE} \\ \text{occurring in } I_b \end{pmatrix} \times \\
&\Bigg[\begin{pmatrix} \text{Probability that} \\ 1 \text{ n}^0 \text{ is emitted} \end{pmatrix} \times \begin{pmatrix} \text{Probability that} \\ 1 \text{ n}^0 \text{ produces} \\ n_1 \text{ n}^0\text{s in } I_b^c \end{pmatrix} \times \begin{pmatrix} \text{Probability of subsequent SEs} \\ \text{occurring in } I_b^c, \text{ resulting in} \\ m = n - n_1 \text{ n}^0\text{s at } t \end{pmatrix} \\
&+ \begin{pmatrix} \text{Probability that} \\ 2 \text{ n}^0\text{s are emitted} \end{pmatrix} \times \begin{pmatrix} \text{Probability those} \\ 2 \text{ n}^0\text{s produce} \\ n_1, n_2 \text{ n}^0\text{s in } I_b^c \end{pmatrix} \times \begin{pmatrix} \text{Probability of subsequent SEs} \\ \text{occurring in } I_b^c, \text{ resulting in} \\ m = n - n_1 - n_2 \text{ n}^0\text{s at } t \end{pmatrix} \\
&\vdots \\
&+ \begin{pmatrix} \text{Probability that} \\ \nu_m^S \text{ n}^0\text{s are emitted} \end{pmatrix} \times \begin{pmatrix} \text{Probability those} \\ \nu_m^S \text{ n}^0\text{s produce} \\ n_1, \ldots, n_{\nu_m^S} \text{ n}^0\text{s in } I_b^c \end{pmatrix} \times \begin{pmatrix} \text{Probability of subsequent SEs} \\ \text{occurring in } I_b^c, \text{ resulting in} \\ m = n - n_1 - \ldots - n_{\nu_m^S} \text{ n}^0\text{s at } t \end{pmatrix} \Bigg].
\end{aligned} \tag{4.77}$$

Just as before, we can easily define the probability of a source event occurring in the short time Δt_o by recalling that the source, S, is defined as 'the probability of a source event occurring per unit time', which results in the following:

$$\begin{pmatrix} \text{Probability of a SE} \\ \text{occurring in } I_b \end{pmatrix} = S(t_o)\Delta t_o \tag{4.78}$$

Next, we may define the complement of Eq. 4.78 using the conservation of probability to find:

$$\begin{pmatrix} \text{Probability of no SE} \\ \text{occurring in } I_b \end{pmatrix} = 1 - S(t_o)\Delta t_o. \tag{4.79}$$

In the event of a SE, we need to consider the probability of ν-tuplet emission, given by

$$\begin{pmatrix}\text{Probability that}\\ \nu\ \text{n}^0\text{s are emitted}\end{pmatrix} = q_\nu^S. \tag{4.80}$$

Next, we need to consider the events that may occur in I_b^c that will result in n neutrons at t. Let us first consider the 'probability of subsequent SEs occurring in I_b^c resulting in n n^{0}s at t,' which is given by $\Theta_n(t|t_o+\Delta t_o)$. Similarly, the 'probability of subsequent SEs occurring in I_b^c resulting in m neutrons at t' is $\Theta_m(t|t_o+\Delta t_o)$.

Finally, we must consider the progeny of the SE that occurred in I_b. For the case of a single neutron produced in the first SE, that neutron is born at time $t_o+\Delta t_o$, propagates in I_b^c, and eventually results in $n_1 = n-m$ neutrons at t. The given probability of this outcome is simply $P_{n_1}(t|t_o+\Delta t_o)$, the single chain solution. For 2 neutrons emitted in the first SE, each of those neutrons is born at $t_o+\Delta t_o$ and will result in two branches with populations n_1, n_2 at t such that $n = m+n_1+n_2$ with probabilities $P_{n_1}(t|t_o+\Delta t_o)$ and $P_{n_2}(t|t_o+\Delta t_o)$. As there could be many combinations of n_1, n_2, and m that satisfy $n = m+n_1+n_2$, we must sum over all these combinations to find:

$$\begin{pmatrix}\text{Probability the 2 n}^0\text{s produce } n_1, n_2\\ \text{n}^0\text{s, such that } m+n_1+n_2 = n, \text{ in } I_b^c\end{pmatrix} = \sum_{m+n_1+n_2=n} \Theta_m(t|t_o+\Delta t_o) P_{n_1}(t|t_o+\Delta t_o) P_{n_2}(t|t_o+\Delta t_o), \tag{4.81}$$

where the sum is actually a triple sum but we leave it as is for convenience. For the case of ν neutrons emitted, the above logic holds and we would have the same structure as above but with a product of $P_{n_1}, \dots P_{n_\nu}$. Thus, to find the entire bracketed term of Eq. 4.77, we sum from $\nu = 0$ to $\nu = \nu_m^S$ to find:

$$\sum_{\nu=0}^{\nu_m^S} q_\nu^S \sum_{m+n_1+\dots+n_\nu=n} \Theta_m(t|t_o+\Delta t_o) \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o+\Delta t_o).$$

Assembling these together, we obtain the Chapman-Kolmogorov equation for the first collision interval probability balance describing a neutron source in an infinite medium:

$$\begin{aligned}\Theta_n(t|t_o) = &\Big[1 - S(t_o)\Delta t_o\Big]\Theta_n(t|t_o+\Delta t_o)\\ &+ S(t_o)\Delta t_o \sum_{\nu=0}^{\nu_m^S} q_\nu^S \sum_{m+n_1+\dots+n_\nu=n} \Theta_m(t|t_o+\Delta t_o) \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o+\Delta t_o).\end{aligned} \tag{4.82}$$

Next, we divide by Δt_o and subtract $\Theta_n(t|t_o+\Delta t_o)$ to find:

$$\begin{aligned}-\frac{\Theta_n(t|t_o+\Delta t_o) - \Theta_n(t|t_o)}{\Delta t_o} = &- S(t_o)\Theta_n(t|t_o+\Delta t_o)\\ &+ S(t_o) \sum_{\nu=0}^{\nu_m^S} q_\nu^S \sum_{m+n_1+\dots+n_\nu=n} \Theta_m(t|t_o+\Delta t_o) \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o+\Delta t_o).\end{aligned} \tag{4.83}$$

If we now evaluate the limit as $\Delta t_o \to 0$, the LHS becomes the derivative of $\Theta_n(t|t_o)$ with respect to t_o, and we have:

$$-\frac{\partial \Theta_n(t|t_o)}{\partial t_o} = -S(t_o)\Theta_n(t|t_o) + S(t_o) \sum_{\nu=0}^{\nu_m^S} q_\nu^S \sum_{m+n_1+\dots+n_\nu=n} \Theta_m(t|t_o) \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o) \tag{4.84}$$

with $n = 0, 1, 2, \ldots$. This equation is the backward master equation for the neutron number distribution in the presence of a neutron source in an infinite medium. The 'final' condition, for which there are zero neutrons in the system at time t_o, is given by

$$\lim_{t_o \to t} \Theta_n(t|t_o) = \delta_{n,0} \tag{4.85}$$

where $\delta_{i,j}$ is the Kronecker delta function.

As with the single chain case, we see Eq. 4.84 is substantially more complex than the previous BMEs for a source. We note, however, that this BME is still linear in Θ_n, just like Eq. 3.58. The additional physics create complexities in the single chain solution itself (see Eq. 4.74) and in the branching possibilities from the first source event that occurs in I_b.

4.3.2 Equation for the Probability Generating Function

The Single Chain Backward PGF Equation

We now define the single chain backward PGF:

$$G(z, t|t_o) = \sum_{n=0}^{\infty} z^n P_n(t|t_o), \tag{4.86}$$

where it is clear that the backward PGF has a dependence on the neutron introduction time, $t < t_f$, and this symbolism should be easily distinguishable from the forward PGF, Eq. 4.19, for this reason. To obtain an equation for the single chain backward PGF, we multiply Eq. 4.74 by z^n and sum over all n to find

$$\begin{aligned} -\sum_{n=0}^{\infty} z^n \frac{\partial P_n(t|t_o)}{\partial t_o} = & -\lambda_t(t_o) \sum_{n=0}^{\infty} z^n P_n(t|t_o) + \Big[\lambda_c(t_o) + \lambda_\ell(t_o)\Big] \sum_{n=0}^{\infty} z^n \delta_{n,0} \\ & + \lambda_f(t_o) \sum_{n=0}^{\infty} z^n \sum_{\nu=0}^{\nu_m^f} q_\nu^f \sum_{n_1+\ldots+n_\nu=n} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o). \end{aligned} \tag{4.87}$$

We will simplify term-by-term; the LHS of Eq. 4.87 is then

$$\begin{aligned} -\sum_{n=0}^{\infty} z^n \frac{\partial P_n(t_f|t)}{\partial t} &= -\frac{\partial}{\partial t_o} \sum_{n=0}^{\infty} z^n P_n(t|t_o) \\ &= -\frac{\partial G(z, t|t_o)}{\partial t_o}, \end{aligned} \tag{4.88}$$

and the first term on the RHS is simple to transform

$$-\lambda_t \sum_{n=0}^{\infty} z^n P_n(t|t_o) = -\lambda_t G(z, t|t_o). \tag{4.89}$$

The empty-state contribution is simply

$$\Big[\lambda_c + \lambda_\ell\Big] \sum_{n=0}^{\infty} z^n \delta_{n,0} = \lambda_c + \lambda_\ell \tag{4.90}$$

because the only contributing term in the sum is $n = 0$.

The nonlinear fission branching terms require additional involvement to put into terms of the backward PGF. Observing that the z^n and the sum over n may be pushed through to the combinatorial sum, we analyze the following:

$$\begin{aligned}\mathcal{I}_\nu(z,t|t_o) &= \sum_{n=0}^{\infty} z^n \sum_{n_1+\ldots+n_\nu=n} \prod_{\nu'=1}^{\nu} P_{n_{\nu'}}(t|t_o) \\ &= \sum_{n=0}^{\infty} z^n \sum_{n_1=0}^{\infty} P_{n_1} \sum_{n_2=0}^{\infty} P_{n_2} \cdots \sum_{n_\nu=0}^{\infty} P_{n_\nu}, \quad n_1+n_2+\cdots+n_\nu = n \\ &= \sum_{n_1=0}^{\infty} P_{n_1} \sum_{n_2=0}^{\infty} P_{n_2} \cdots \sum_{n_{\nu-1}=0}^{\infty} P_{n_{\nu-1}} \sum_{n=0}^{\infty} z^n P_{n-(n_1+n_2+\ldots n_{\nu-1})}, \end{aligned} \tag{4.91}$$

where we recognize that as we push the sum over n through each n_i summation, we set the values of the n_i that satisfy the requirement that $\sum_i n_i = n$, and by the pushing through the final n_ν sum, there is only one number that will satisfy the above requirement, and we then lose the sum over n_ν. By assigning a new index $m = n - (n_1 + n_2 + \ldots n_{\nu-1})$, inserting into Eq. 4.91, rearranging, and noting that $P_{m<0} = 0$, we obtain

$$\begin{aligned}\mathcal{I}_\nu(z,t|t_o) &= \sum_{n_1=0}^{\infty} z^{n_1} P_{n_1} \sum_{n_2=0}^{\infty} z^{n_2} P_{n_2} \cdots \sum_{n_{\nu-1}=0}^{\infty} z^{n_{\nu-1}} P_{n_{\nu-1}} \sum_{m=0}^{\infty} z^m P_m \\ &= \Big[G(z,t|t_o)\Big]^\nu. \end{aligned} \tag{4.92}$$

The equation for the backward PGF is finally procured:

$$-\frac{\partial G(z,t|t_o)}{\partial t_o} = -\lambda_t(t_o)G(z,t|t_o) + \lambda_c(t_o) + \lambda_\ell(t_o) + \lambda_f(t_o) \sum_{\nu=0}^{\nu_m^f} q_\nu^f \Big[G(z,t|t_o)\Big]^\nu, \tag{4.93}$$

with the final condition, found by applying Eq. 4.86 to Eq. 4.75, is

$$\lim_{t_o \to t} G(z,t|t_o) = z. \tag{4.94}$$

Equation 4.93 is a nonlinear PDE whose solution may be obtained, for a set value of z, by integrating backward in time starting at $t' = t$ and ending at $t' = t_o$. In the next section, Sec. 4.3.3, we will show how to solve this equation under certain conditions. First, we will introduce the complementary PGF that converts Eq. 4.93 into a more convenient form, and we will then obtain the separate source PGF equations.

As is historically customary, we define the complementary backward single chain PGF

$$\mathcal{G}(z,t|t_o) = 1 - G(z,t|t_o), \tag{4.95}$$

which permits more convenient forms of the backward single chain PGF equation [21, 18]. By inserting Eq. 4.95 into Eq. 4.93, we find

$$\frac{\partial \mathcal{G}(z,t|t_o)}{\partial t_o} = -\lambda_t(t_o)\Big[1 - \mathcal{G}(z,t|t_o)\Big] + \lambda_c(t_o) + \lambda_\ell(t_o) + \lambda_f(t_o) \sum_{\nu=0}^{\nu_m^f} q_\nu^f \Big[1 - \mathcal{G}(z,t|t_o)\Big]^\nu, \tag{4.96}$$

with final condition

$$\lim_{t_o \to t} \mathcal{G}(z,t|t_o) = 1 - z. \tag{4.97}$$

Obviously, this does not immediately provide us with a satisfactory simplification, prompting us to analyze the nonlinear terms. If we apply the Binomial Theorem to the nonlinear terms, we find

$$\begin{aligned}
\sum_{\nu=0}^{\nu_m^f} q_\nu^f \Big[1 - \mathcal{G}(z,t|t_o)\Big]^\nu &= \sum_{\nu=0}^{\nu_m^f} q_\nu^f \sum_{i=0}^{\nu} (-1)^i \frac{\nu!}{(\nu-i)!i!} \big[\mathcal{G}(z,t|t_o)\big]^i \\
&= \sum_{i=0}^{\nu_m^f} \frac{(-1)^i}{i!} \mathcal{G}^i \sum_{\nu=i}^{\nu_m^f} \frac{\nu!}{(\nu-i)!} q_\nu^f \\
&= \sum_{i=0}^{\nu_m^f} \frac{(-1)^i}{i!} \chi_i \mathcal{G}^i,
\end{aligned} \tag{4.98}$$

where we have defined the the factorial moments of the induced fission multiplicity distribution as

$$\chi_i = \sum_{\nu=i}^{\nu_m^f} \frac{\nu!}{(\nu-i)!} q_\nu^f, \tag{4.99}$$

which are identical to the factorial moments, Eq. 4.38, obtained in the process of applying the Quadratic Approximation in Sec. 4.2.4. From this, and using $-\lambda_f = \lambda_c + \lambda_\ell - \lambda_t$, we obtain an equation for $\mathcal{G}$ in the desired form

$$\frac{\partial \mathcal{G}(z,t|t_o)}{\partial t_o} = \lambda_t(t_o)\mathcal{G}(z,t|t_o) + \lambda_f(t_o)\left[-1 + \sum_{\nu=0}^{\nu_m^f} \frac{(-1)^\nu}{\nu!} \chi_\nu \Big[\mathcal{G}(z,t|t_o)\Big]^\nu\right], \tag{4.100}$$

with final condition given by Eq. 4.97. Equation 4.100 is in a useful form because we will be interested in specific probability quantities, such as the survival probability. The survival probability is the probability that a single neutron chain has survived up to a certain point in time and is useful in quantifying how safe a reactor might be. To avoid a lengthy digression, but to justify the introduction of Eq. 4.95, we simply point out that the survival probability may be extracted from $\mathcal{G}$ by setting $z = 0$, such that $\mathcal{G}(0,t|t_o) = P_S(t|t_o)$, and the form of Eq. 4.95 does not change.

The Source Backward PGF Equation

For a constant randomly emitting neutron source, we define the PGF as:

$$H(z,t|t_o) = \sum_{n=0}^{\infty} z^n \Theta_n(t|t_o). \tag{4.101}$$

Multiplying Eq. 4.84 by z^n, summing over all n, and applying similar manipulations as the single chain case, we find H to satisfy the linear PDE:

$$-\frac{\partial H(z,t|t_o)}{\partial t_o} = S(t_o)\left[-1 + \sum_{\nu=0}^{\nu_m^S} q_\nu^S \big[G(z,t|t_o)\big]^\nu\right] H(z,t|t_o), \tag{4.102}$$

with final condition given by

$$\lim_{t_o \to t} H(z,t|t_o) = 1. \tag{4.103}$$

4.3.3 Solutions to the PGF PDE

Single Chain

Equation 4.100 can be solved using the MoC (with some approximations), and we obtain the characteristic system by writing down the total derivative of $\mathcal{G}$ with respect to t_o:

$$\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}t_o} = \frac{\partial \mathcal{G}}{\partial z}\frac{\mathrm{d}z}{\mathrm{d}t_o} + \frac{\partial \mathcal{G}}{\partial t_o}. \tag{4.104}$$

Comparing this expression to Eq. 4.100, we may extract the characteristic system:

$$\frac{\mathrm{d}z}{\mathrm{d}t_o} = 0 \tag{4.105a}$$

$$\frac{\mathrm{d}\mathcal{G}}{\mathrm{d}t_o} = \lambda_t(t_o)\mathcal{G}(z,t|t_o) - \lambda_f(t_o) + \lambda_f(t_o)\sum_{\nu=0}^{\nu_m^f}\frac{(-1)^\nu}{\nu!}\chi_\nu\Big[\mathcal{G}(z,t|t_o)\Big]^\nu. \tag{4.105b}$$

Equation 4.105a informs us that z is a constant along the characteristic and therefore not a function of t_o.

At first glance, Eq. 4.105b does not provide much information, but we have at least simplified the PDE to an ODE as a start. This is where we must once again employ the Quadratic Approximation to coax out a solution for $\mathcal{G}$. In the Forward Formulation (FF), the QA was applied to the characteristic ODE for $\mathrm{d}z/\,\mathrm{d}t$, Eq. 4.34a, but we do not have such an equation here (because $\mathrm{d}z/\,\mathrm{d}t_o = 0$). Instead for the Backward Formulation (BF), we must apply a truncation to the equation for $\mathcal{G}$, the single chain PGF solution. This is an interesting correspondence that is worth mentioning here. For the FF, the PGF PDE, Eq. 4.30, has single chain physics and source physics encapsulated in a single equation and the single chain effects are expressed in the coefficient of $\partial G/\,\partial z$, given by $g(z,t)$ (Eq. 4.32). Additionally, the FF characteristic equation for the solution, $\mathrm{d}G/\,\mathrm{d}z$, has the source physics with the single chain physics folded into the integral of Eq. 4.45. For the BF, the single chain physics are completely encapsulated in the entire PGF PDE, Eq. 4.100, with a separate PGF PDE for H, Eq. 4.102, to account for source effects (with the single chain physics once again folded in). With this is mind, this correspondence is expected as it is by design how the two formulations are related.

Proceeding, the QA for the BF is applied by truncating the nonlinear summation of Eq. 4.105b at second order, i.e., set $\nu_m^f = 2$ in the upper limit. As we mentioned in the FF QA, we must remain cautious that we are not setting $\nu_m^f = 2$ in our data and we can (and should) still use the entire multiplicity distribution to calculate χ_2. Doing so, Eq. 4.105b becomes:

$$\frac{\mathrm{d}\mathcal{G}(z,t|t_o)}{\mathrm{d}t_o} = \lambda_t\mathcal{G}(z,t|t_o) - \lambda_f + \lambda_f\chi_0 - \lambda_f\chi_1\mathcal{G} + \frac{\lambda_f\chi_2}{2}\mathcal{G}^2, \tag{4.106}$$

which can be simplified by recalling $\chi_0 = 1$, $\chi_1 = \overline{\nu}$, $\chi_2' = \lambda_f\chi_2$, and $\lambda_t - \overline{\nu}\lambda_f = -\alpha$ to find

$$-\frac{\mathrm{d}\mathcal{G}(z,t|t_o)}{\mathrm{d}t_o} = \alpha(t_o)\mathcal{G}(z,t|t_o) - \frac{\chi_2'(t_o)}{2}\big[\mathcal{G}(z,t|t_o)\big]^2. \tag{4.107}$$

Equation 4.107 is immediately recognized as a second-order Bernoulli ODE (a homogeneous Riccati equation) which has an analytical solution. Introducing the transformation $y = 1/\mathcal{G}$, Eq. 4.107 is reduced to an inhomogeneous linear first-order ODE

$$\frac{\mathrm{d}y(z,t|t_o)}{\mathrm{d}t_o} = \alpha(t_o)y(z,t|t_o) - \frac{\chi_2'(t_o)}{2}, \tag{4.108}$$

which is quickly solved using the integrating factor technique and integrating backwards in time. We eventually arrive at an expression for $\mathcal{G}$:

$$\begin{aligned}\frac{1}{\mathcal{G}(z,t|t_o)} &= \frac{1}{\mathcal{G}(z,t|t)}\exp\left\{\int_t^{t_o}\mathrm{d}t'\alpha(t')\right\} - \int_t^{t_o}\mathrm{d}t'\frac{\chi_2'(t')}{2}\exp\left\{\int_{t'}^{t_o}\mathrm{d}t''\alpha(t'')\right\} \\ &= \frac{1}{1-z}a_o(t|t_o) - b_o(t|t_o)\end{aligned} \tag{4.109}$$

where we have inserted the final condition $\mathcal{G}(z,t|t_o=t) = 1-z$ and we have defined

$$\begin{aligned}a_o(t|t_o) &= \exp\left\{\int_t^{t_o}\mathrm{d}t'\alpha(t')\right\} \\ &= \exp\left\{-\int_{t_o}^{t}\mathrm{d}t'\alpha(t')\right\}\end{aligned} \tag{4.110a}$$

$$\begin{aligned}b_o(t|t_o) &= \int_t^{t_o}\mathrm{d}t'\frac{\chi_2'(t')}{2}\exp\left\{\int_{t'}^{t_o}\mathrm{d}t''\alpha(t'')\right\} \\ &= -\int_{t_o}^{t}\mathrm{d}t'\frac{\chi_2'(t')}{2}\exp\left\{-\int_{t_o}^{t'}\mathrm{d}t''\alpha(t'')\right\}\end{aligned} \tag{4.110b}$$

which can be thought of as the backward analogs to Eqs. 4.44a and 4.44b. With that said, we state the relationship between the forward a, b and backward a_o, b_o:

$$a_o(t|t_o) = \frac{1}{a(t)} \tag{4.111a}$$

$$\begin{aligned}b_o(t|t_o) &= -a_o(t|t_o)b(t) \\ &= -\frac{a(t)}{b(t)}.\end{aligned} \tag{4.111b}$$

From this, we may write the backward $\mathcal{G}$ in terms of the forward coefficients a, b:

$$\frac{1}{\mathcal{G}(z,t|t_o)} = \frac{1}{a(t)}\left[\frac{1}{1-z} + b(t)\right]. \tag{4.112}$$

Reverting to the original PGF, we obtain a solution to Eq. 4.93, in the Quadratic Approximation:

$$\begin{aligned}G(z,t|t_o) &= 1 - \frac{1}{\frac{a_o(t|t_o)}{1-z} - b_o(t|t_o)} \\ &= 1 + \frac{a(t)}{\frac{1}{z-1} - b(t)},\end{aligned} \tag{4.113}$$

which is clearly equivalent to forward solution for G given by Eq. 4.47.

Source

Equation 4.102 is a linear separable PDE which which is easily solved by integrating backwards in time to find a closed-form expression of H which is dependent on the single chain PGF, G,

$$H(z,t|t_o) = \exp\left\{-\int_t^{t_o}\mathrm{d}t'\,S(t')\left[-1 + \sum_{\nu=0}^{\nu_m^S} q_\nu^S\left[G\left(z,t|t'\right)\right]^\nu\right]\right\}. \tag{4.114}$$

From Eq. 4.114, we may insert the single chain PGF, G, and then attempt to evaluate the integral in the exponential. We consider the source to be constant in time and singlet emitting, i.e. $q_\nu^S = \delta_{\nu,1}$, such that we only have a first-order power of G as part of the integrand. This reduces Eq. 4.114 accordingly:

$$H(z,t|t_o) = \exp\left\{-S\int_t^{t_o} \mathrm{d}t' \big[G(z,t|t') - 1\big]\right\}. \tag{4.115}$$

Noting Eq. 4.113 solved for $G-1$, we may rewrite Eq. 4.115 as $H = \exp\{+SI\}$, where I is the integral of $-(G-1)$. The integral in the exponential is computable if we assume that χ_2' is constant with respect to time. For such a case, the integral takes the form:

$$\begin{aligned} I &= \int_t^{t_o} \mathrm{d}t' \left[\frac{1}{1-z}a_o(t|t') - b_o(t|t')\right]^{-1} \\ &= (1-z)\int_t^{t_o} \mathrm{d}t' \frac{1/a_o(t|t')}{1-(1-z)\frac{b_o(t|t')}{a_o(t|t')}}, \end{aligned}$$

where we keep the notation in terms of the backward a_o, b_o to give the reader the full 'backward experience'. The ratio in the denominator can be simplified as follows:

$$\begin{aligned} \frac{b_o(t|t')}{a_o(t|t')} &= \frac{\chi_2'}{2}\exp\left\{-\int_t^{t'}\mathrm{d}x\alpha(x)\right\}\int_t^{t'}\mathrm{d}w\exp\left\{\int_w^{t'}\mathrm{d}x\alpha(x)\right\} \\ &= \frac{\chi_2'}{2}\int_t^{t'}\mathrm{d}w\frac{1}{a_o(t|w)}. \end{aligned} \tag{4.116}$$

Then, by making the substitutions $j_o(t|t') = \exp\{-\int_t^{t'}\mathrm{d}x\alpha(x)\} = 1/a_o(t|t')$ and $J_o(t|t') = \int_t^{t'}\mathrm{d}x j_o(t|x)$, the integral inherits a simplistic form:

$$\begin{aligned} I &= (1-z)\int_t^{t_o}\mathrm{d}t'\frac{j_o(t|t')}{1-(1-z)\frac{\chi_2'}{2}\int_t^{t'}\mathrm{d}t'' j_o(t|t'')} \\ &= (1-z)\int_0^{J_o(t|t_o)}\mathrm{d}J_o\frac{1}{1-(1-z)\frac{\chi_2'}{2}J_o} \\ &= -\frac{2}{\chi_2'}\ln\left[1-(1-z)\frac{\chi_2'}{2}\int_t^{t_o}\mathrm{d}t'\frac{1}{a_o(t|t')}\right]. \end{aligned}$$

This leads to a solution to the backward PGF equation for a singlet emitting source where we applied the QA to obtain the supplementary single chain PGF solution:

$$\begin{aligned} H(z,t|t_o) &= \left(1-(1-z)\frac{b_o(t|t_o)}{a_o(t|t_o)}\right)^{-\eta} \\ &= \Big[1-(z-1)b(t)\Big]^{-\eta} \end{aligned} \tag{4.117}$$

where $\eta = 2S/\chi_2'$ and we used Eqs. 4.111 to express H in terms of the forward coefficient b; from which we see the second line of Eq. 4.117 is exactly equivalent to Eq. 4.53 for the forward source PGF. Given these solutions for the single chain and in the presence of a source, Eqs. 4.113 and 4.117, respectively, we are now prepared to invert these expressions to obtain the neutron number PDFs.

4.3.4 Inversion of the PGF

In this section, we show how to invert the expressions we obtained for the backward PGFs in the Quadratic Approximation. The process is the same as in Sec. 4.2.6 for which we inverted the forward PGF expressions. We will keep the notation in the backward coefficients for a_o, b_o to give the reader the backward perspective.

Single Chain

To invert the backward PGF for an individual neutron chain, we begin by rearranging Eq. 4.113:

$$\begin{aligned} G(z,t|t_o) &= 1 - \frac{1-z}{a_o(t|t_o) - (1-z)b_o(t|t_o)} \\ &= \frac{a_o + |b_o| - 1}{a_o + |b_o|(1-z)} - \frac{(1-|b_o|)z}{a_o + |b_o|(1-z)} \\ &= \frac{a_o + |b_o| - 1}{a_o + |b_o|}\left[1 - \frac{|b_o|}{a_o + |b_o|}z\right]^{-1} - \frac{(1-|b_o|)z}{a_o + |b_o|}\left[1 - \frac{|b_o|}{a_o + |b_o|}z\right]^{-1} \end{aligned} \tag{4.118}$$

where $a_o(t|t_o)$ and $b_o(t|t_o)$ are defined by Eqs. 4.110a and 4.110b, respectively, and we have taken advantage of the fact that $b_o(t|t_o) < 0$ for all $t_o < t$. By expanding the bracketed terms of Eq. 4.118 into a Taylor series about $z = 0$, pushing the z factor of the second term into the expansion and shifting the index appropriately, we find

$$\begin{aligned} G(z,t|t_o) &= \frac{a_o + |b_o| - 1}{a_o + |b_o|}\sum_{n=0}^{\infty}\left(\frac{|b_o|}{a_o + |b_o|}\right)^n z^n - \frac{1-|b_o|}{a_o + |b_o|}\sum_{n=1}^{\infty}\left(\frac{|b_o|}{a_o + |b_o|}\right)^{n-1} z^n \\ &= \frac{a_o + |b_o| - 1}{a_o + |b_o|} + \frac{a_o}{|b_o|(a_o + |b_o|)}\sum_{n=1}^{\infty}\left(\frac{|b_o|}{a_o + |b_o|}\right)^n z^n. \end{aligned} \tag{4.119}$$

By comparing Eq. 4.119 to the definition: $G(z,t|t_o) = \sum_{n=0}^{\infty} P_n(t|t_o)z^n$, we find the extinction probability has been naturally separated and the remainder of the distribution is extracted by inspection to find:

$$\begin{aligned} P_0(t|t_o) &= 1 - \frac{1}{a_o(t|t_o) - b_o(t|t_o)} \\ &= 1 - \frac{a(t)}{1 + b(t)} \end{aligned} \tag{4.120a}$$

$$\begin{aligned} P_n(t|t_o) &= a_o(t|t_o)\frac{[|b_o(t|t_o)|]^{n-1}}{[a_o(t|t_o) - b_o(t|t_o)]^{n+1}} \\ &= \frac{a(t)}{\big[1 + b(t)\big]^2}\left[\frac{b(t)}{1 + b(t)}\right]^{n-1} \end{aligned} \tag{4.120b}$$

where $n = 1, 2, 3, \ldots$ in Eq. 4.120b and we have transformed the solution to the forward coefficients a, b to demonstrate the functional equivalence between the two formulation's end results.

Equations 4.120a and 4.120b constitute the discrete neutron number distribution for a single neutron chain obtained from the complementary PGF equation in the Quadratic Approximation. Recalling that the operational variable in the backward formulation is the time the initial neutron is injected, we see that, from Eqs. 4.110a and 4.110b, the limits $\lim_{t_o \to t} a_o(t|t_o) = 1$ and $\lim_{t_o \to t} b_o(t|t_o) = 0$. From these limits, the final condition imposed on the distribution is satisfied because $\lim_{t_o \to t} P_0(t|t_o) = 0$ and $\lim_{t_o \to t} P_n(t|t_o) = \delta_{n,1}$ (using the identity $0^0 = 1$).

Table 4.1: Fast neutron (14 MeV) multiplicity distribution data for a ^{235}U metal system. Data taken from [42].

q_0^f	q_1^f	q_2^f	q_3^f	q_4^f	q_5^f	q_6^f	q_7^f	$\overline{\nu}$	$\overline{\nu^2}$	χ_2	χ_3
0.00	0.009	0.022	0.179	0.310	0.310	0.11	0.06	4.47	21.318	16.92	53.2

Table 4.2: Fast neutron data for a ^{235}U metal system.

$N\ [b^{-1}cm^{-1}]$	$\sigma_f\ [b]$	$\sigma_c\ [\mu b]$	$v\ [cm/s]$	k	$\tau\ [ns]$	$\lambda_f\ [1/s]$	$\alpha\ [1/s]$
0.05088	2.053	889.7	$5.174 \cdot 10^9$	4.47	1.849	$5.4050 \cdot 10^8$	$1.822 \cdot 10^9$

In the Presence of a Source

To obtain the number distribution in the presence of a source, we begin with Eq. 4.117:

$$H(z,t|t_o) = \left(1-(1-z)\frac{b_o(t|t_o)}{a_o(t|t_o)}\right)^{-\eta}.$$

After rearranging and defining $c_o(t|t_o) = b_o(t|t_o)/a_o(t|t_o)$, where we also note that $c_o < 0$ because $b_o < 0$ for all $t_o < t$ regardless of criticality, we find:

$$\begin{aligned} H(z,t|t_o) &= \Big[1-(1-z)c_o(t|t_o)\Big]^{-\eta} \\ &= \Big[1+|c_o(t|t_o)|\Big]^{-\eta}\left[1-\frac{|c_o(t|t_o)|}{1+|c_o(t|t_o)|}z\right]^{-\eta}. \end{aligned} \tag{4.121}$$

Upon expanding the bracketed factor of Eq. 4.121, we obtain:

$$H(z,t|t_o) = \Big[1+|c_o(t|t_o)|\Big]^{-\eta}\sum_{n=0}^{\infty}\frac{\Gamma(\eta+n)}{n!\Gamma(\eta)}\left[\frac{|c_o(t|t_o)|}{1+|c_o(t|t_o)|}\right]^n z^n, \tag{4.122}$$

and we can therefore determine the number distribution in the presence of a source by comparing to the original definition, $H(z,t|t_o) = \sum_{n=0}^{\infty}\Theta_n(t|t_o)z^n$, to find

$$\begin{aligned} \Theta_n(t|t_o) &= \left[1+\frac{|b_o(t|t_o)|}{a_o(t|t_o)}\right]^{-\eta}\frac{\Gamma(\eta+n)}{n!\Gamma(\eta)}\left[\frac{|b_o(t|t_o)|}{a_o(t|t_o)+|b_o(t|t_o)|}\right]^n \\ &= \frac{1}{(1+b(t))^{\eta}}\left[\frac{\Gamma(\eta+n)}{n!\Gamma(\eta)}\right]\cdot\left[\frac{b(t)}{1+b(t)}\right]^n, \end{aligned} \tag{4.123}$$

with $n = 0, 1, 2, \ldots$ and we have once again converted the expression in terms of the forward coefficients a, b to show the equivalence to Eq. 4.61. With Eqs. 4.120 and 4.123, we have derived the neutron number distribution for a single chain and in the presence of a source in the Quadratic Approximation from the backward master equations.

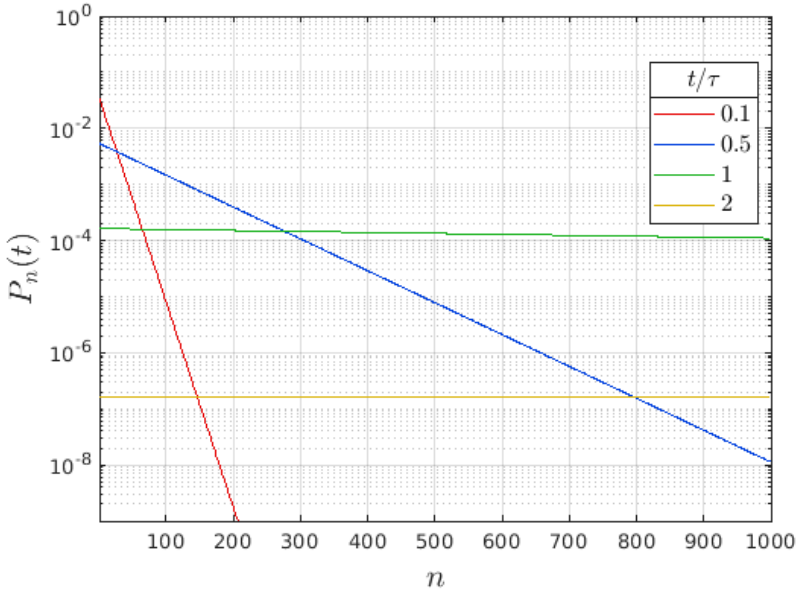


Figure 4.4: Single chain fast neutron number distributions at different times for a ^{235}U system. Extinction probabilities are $P_0(0.1\tau) = 0.5420$, $P_0(0.5\tau) = 0.5819$, $P_0(\tau) = 0.5894$, and $P_0(2\tau) = 0.5896$.

4.4 Analysis, Discussion, and the Survival Probability

We now consider a system composed of pure ^{235}U metal with a full multiplicity distribution seen in Table 4.1 for fast neutrons of 14 MeV, where we have included the first three factorial moments. For such a system $\overline{\nu} = 4.47$, which is drastically different from the BFM from the previous chapter with $\overline{\nu} = 2$ because fast neutrons are prone to cause more neutrons to emerge from an IFE due to the amount of energy delivered to the nucleus on impact. We include χ_2 because we will use it for the QA calculations and we include χ_3 to give the reader a sense of the growth of the factorial moments of the multiplicity distribution.

From the simple comparison of the full multiplicity distribution $\overline{\nu} = 4.47$ and the BFM $\overline{\nu} = 2$, we should expect the number distributions to vary from the previous chapter's example in Sec. 3.4. Figure 4.4 shows the single chain fast neutron number distribution for such a system at different times. This system is highly supercritical ($k = 4.47$ because σ_c is much smaller than σ_f) and, as expected, the chain grows large very quickly which is exemplified by the flattening of the distribution to accommodate the probabilities for larger n values. By analyzing the long-time asymptotic behavior of the chains, the flattening can be analyzed to obtain useful probabilistic quantities that help to characterize a system. The most important quantities are known as the survival probability of a given chain and the probability of initiation. We will now walk through the probabilistic thought process to formally define these probabilities.

First we note that the single chain number distribution always has the extinction probability, $P_0(t)$, readily separated from the distribution's analytical expression (see Eqs. 4.57 and 4.120). Knowing P_0 allows us to compute the total probability that the chain has *not* gone extinct, or has survived, up to time t which is called the *survival probability*, $P_S(t)$. We do this by noting the

normalization condition:

$$1 = \sum_{n=0}^{\infty} P_n(t) = P_0(t) + \sum_{n=1}^{\infty} P_n(t), \tag{4.124}$$

and as was just mentioned, $P_S(t)$ is simply the probability that the chain has not gone extinct and is therefore the probability of there being a non-zero number of neutrons in the system at a given time, i.e.,

$$P_S(t) = \sum_{n=1}^{\infty} P_n(t). \tag{4.125}$$

From Eqs. 4.124, 4.125, and 4.57a, a useful expression for the survival probability is obtained:

$$P_S(t) = 1 - P_0(t) = \frac{a(t)}{1 + b(t)}. \tag{4.126}$$

If we then consider a neutron that is injected into the system at a time t_o and evaluate the limit as $t \to \infty$ of Eq. 4.126, we obtain the probability that said neutron will initiate an indefinitely persistent chain reaction[1], i.e. a divergent chain. This probability is given by:

$$\lim_{t\to\infty} P_S(t) = \left[\mathrm{e}^{-\int_{t_o}^{\infty} \mathrm{d}t' \alpha(t')} + \int_{t_o}^{\infty} \mathrm{d}t' \frac{\chi_2'(t')}{2} \exp\left\{ - \int_{t_o}^{t'} \mathrm{d}t'' \alpha(t'') \right\} \right]^{-1}, \tag{4.127}$$

If the system is subcritical, i.e. $\alpha < 0$, the first term in Eq. 4.127 will diverge and $\lim_{t\to\infty} P_S(t) = 0$, which tells us $P_0(\infty) = 1$ and therefore the chain is guaranteed to extinguish. This is a self-consistent statement that if the multiplication factor $k < 1$, then each successive generation of a neutron chain is on average smaller than the preceding generation, thus in such a scenario one is guaranteed that chain will eventually diminish. For a supercritical system with $\alpha > 0$, the first term of Eq. 4.127 decays to zero and the limit of P_S takes on some non-zero value, which may be written more compactly as

$$\lim_{t\to\infty} P_S(t) = \left[\int_{t_o}^{\infty} \mathrm{d}t' \frac{\chi_2'(t')}{2} \exp\left\{ - \int_{t_o}^{t'} \mathrm{d}t'' \alpha(t'') \right\} \right]^{-1}. \tag{4.128}$$

If we were to consider time-independent α and χ_2', we have from Eqs. 4.44: $a(t) = \exp\{\alpha t\}$ and $b(t) = \frac{\chi_2'}{2\alpha}[\exp\{\alpha t\} - 1]$, where we have set $t_o = 0$. The example ^{235}U system we are considering is supercritical, and therefore as time progresses we find (with α and χ_2' constant):

$$\lim_{t\to\infty} P_S(t) = \frac{2\alpha}{\chi_2'}. \tag{4.129}$$

Equation 4.129 informs us that after a long period of time, the neutron chain has a probability of never going extinct given by $2\alpha/\chi_2'$. We will come back to this quantity shortly with an informed perspective.

Up to now, we have yet to explain the flattening seen in Fig. 4.4 for a supercritical system as time progresses. We just showed that, in a supercritical system, the chain will not go extinct with probability $2\alpha/\chi_2'$ (or use Eq. 4.128 for general time-dependence). However, if we evaluate the limit as $t \to \infty$ of any particular number n of the distribution using Eq. 4.57b, we find:

$$\lim_{t\to\infty} P_n(t) = \lim_{t\to\infty} \frac{a(t)}{(1 + b(t))^2} \left[\frac{b(t)}{1 + b(t)} \right]^{n-1} \sim \frac{1}{\exp\{\alpha t\}} = 0, \quad \text{for } 1 \le n < \infty. \tag{4.130}$$

[1] If we were analyzing the backward equations, we would take the limit as $t_o \to -\infty$, which is to say we inject the initial neutron in the infinite past and observe the distribution at time t.

Thus, for any $n \in [1, \infty)$, the probability of any particular number of neutrons existing within the system goes to zero- this is why the distribution flattens and continually decreases. Perhaps this result does not sit well with reader because we have just shown the $P_n \to 0$ as $t \to \infty$ for all n, while we have also shown that the chain will also continue to grow indefinitely with probability $2\alpha/\chi_2'$. This can be explained by once again considering the normalization condition now evaluated at $t = \infty$:

$$1 = \sum_{n=0}^{\infty} P_n(\infty) = P_0(\infty) + P_1(\infty) + P_2(\infty) + \cdots + P_\infty(\infty). \tag{4.131}$$

This expression can be simplified by using Eq. 4.130, which tells us $P_1(\infty) = P_2(\infty) = \ldots = 0$ and Eq. 4.128 which provides $P_0(\infty) = 1 - \lim_{t\to\infty} P_S(t)$ (or $P_0(\infty) = 1 - 2\alpha/\chi_2'$ for constant α, χ_2'). Using these in Eq. 4.131 provides an expression for the probability of there being an infinite number of neutrons in the system at $t = \infty$, $P_\infty(\infty)$:

$$P_\infty(\infty) = \left[\int_{t_o}^{\infty} \mathrm{d}t' \frac{\chi_2'(t')}{2} \exp\left\{ - \int_{t_o}^{t'} \mathrm{d}t'' \alpha(t'') \right\} \right]^{-1}, \tag{4.132}$$

which is clearly identical to Eq. 4.128. For constant α, χ_2', we obtain the expression:

$$P_\infty(\infty) = \frac{2\alpha}{\chi_2'} = 2\frac{k-1}{k} \cdot \frac{\overline{\nu}}{\overline{\nu^2} - \overline{\nu}}. \tag{4.133}$$

Here we have used $\alpha = (k-1)/\tau$ and $\chi_2' = \lambda_f \chi_2$ with $\lambda_f = p_f/\tau = k/(\overline{\nu}\tau)$ and $\chi_2 = \overline{\nu^2} - \overline{\nu}$. With Eq. 4.133, we have found that a neutron chain has a non-zero probability of growing in infinitude and for this reason we call $P_\infty(\infty)$ the *probability of divergence* or, more commonly, the *probability of initiation* (POI) for a single neutron chain. This agrees with our intuition that a supercritical system will, on average, produce chains that continue to grow with each successive generation. We note that the POI is not necessarily equal to one, i.e., divergence is not a certainty, and there is a complementary probability that the chain will eventually extinguish given by $P_0(\infty) = 1 - P_\infty(\infty)$.

We show the POI as a function of k in Fig. 4.5, where we note that when $k < 1$ the POI is zero (Eq. 4.133 will give a negative value because $\alpha < 0$, so be cautious when interpreting this result). Intuitively, this can be explained because, on average, a generation's population is less than the previous generation's population and therefore a chain is guaranteed to perish on a long enough timeline in a subcritical system- thus, no divergence. This is also explained mathematically by recognizing that $\alpha \equiv 0$ for an exactly critical system and $\alpha < 0$ for subcritical systems; therefore $a(t) = \exp\{-|\alpha|t\}$, $b(t) = \frac{\chi_2'}{2|\alpha|}[1 - \exp\{-|\alpha|t\}]$, and the limit of $P_\infty(\infty) = \lim_{t\to\infty} P_S(t) = 0$ (this also tells us that $P_0(\infty) = 1$ and extinction is guaranteed). For the supercitical regime, Fig. 4.5 demonstrates the POI increases approximately linearly for $k \in [1, 2]$ and the POI approaches 1 as $k \to \infty$. Figure 4.6 shows the effect of differing criticality on the single chain number distribution at different instances in time. The POIs for these systems are $P_\infty(\infty)|_{k=0.89} = 0$, $P_\infty(\infty)|_{k=0.99} = 0$, and $P_\infty(\infty)|_{k=1.12} = 0.014$. For a short period of time, around $t = \tau$ (Fig. 4.6a), the distributions vary only slightly from one another. This is mostly due to the 'speed limit' of the neutron interactions, i.e., the neutrons are moving at a finite speed and thus physically the chain can only be so large. Figure 4.6b shows the distributions at a later time of $t = 10\tau$ where we see the subcritical system of $k = 0.89$ has chains that will most likely have extinguished while the $k = 0.99$ system will have some chains that are more likely to still be propagating. This is an interesting feature for systems with $k \lessapprox 1$, where a chain has the potential to persist for very long time periods before eventually going extinct.

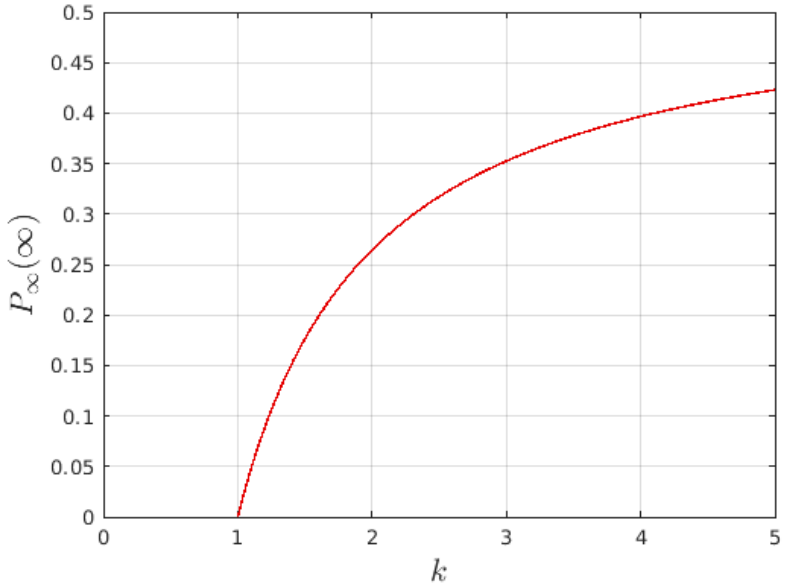
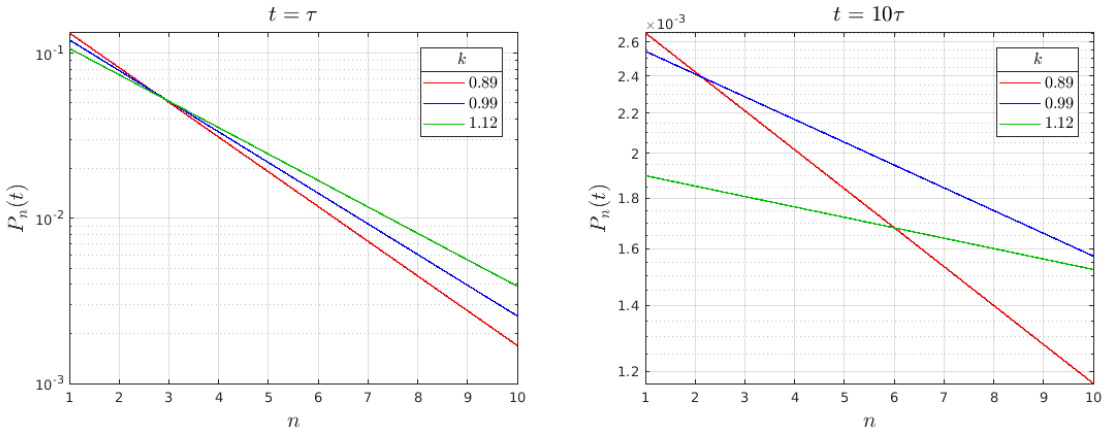


Figure 4.5: The single chain POI as a function of system criticality.



(a) $P_0(\tau)|_{k=0.89} = 0.655$, $P_0(\tau)|_{k=0.99} = 0.654$, $P_0(\tau)|_{k=1.12} = 0.653$.

(b) $P_0(10\tau)|_{k=0.89} = 0.970$, $P_0(10\tau)|_{k=0.99} = 0.951$, $P_0(10\tau)|_{k=1.12} = 0.921$.

Figure 4.6: Single chain number distributions for varying criticality with corresponding P_0 written underneath each plot.

We next consider the case with a singlet-emitting source in a ^{235}U system with the Quadratic Approximation applied to the single chain physics and thus Eq. 4.61 may be used (or Eq. 4.123). Figure 4.7 shows the number distributions due to varying source strengths, given in terms of $\eta = S/\frac{1}{2}\chi_2'$, for this supercritical system. As was seen in Fig. 3.5 for the BFM case, the number distribution undergoes a qualitative change from a monotonically decreasing distribution for $\eta < 1$

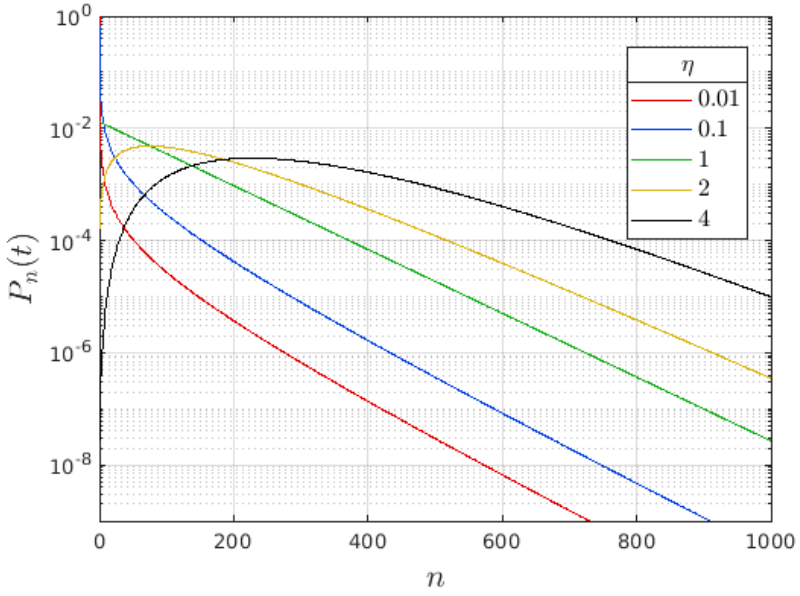


Figure 4.7: Neutron number distributions due to singlet-emitting sources of different strengths at a given time.

to a unimodal distribution when $\eta > 1$. As was observed by Prinja & Souto [16], this corresponds to the system transitioning from a stochastic system towards a more deterministic one. One must remain wary that $\eta > 1$ does not mean the system should be treated deterministically but, rather, that the source is considered 'strong' and produces a number distribution with lower dispersion about the mean (i.e., the ratio of the variance to the mean decreases)[2]. A metric for when to treat a system stochastically or deterministically has been proposed by Méchitoua which involves the total population of the chain and is given in terms of a population cutoff, C. The cutoff is provides an estimate for when a chain will almost certainly persist in perpetuity (i.e., diverge) and can be

[2]To add additional explanation, one may consider the difference of the mode to the mean of the distribution. For a single chain, the mode $M(t)$ (i.e., the n value that occurs with the greatest frequency and therefore has the highest probability) is

$$M(t) = \begin{cases} 0 \text{ if } P_0(t) > P_1(t) \\ 1 \text{ if } P_0(t) < P_1(t) \end{cases}$$

because $P_1(t) > P_n(t)$ for any $n > 1$ at a given time (even if that difference is imperceptibly small) except in the infinite limit when $M(\infty) = 0, \infty$ depending on which probability, $P_0(\infty)$ or $P_\infty(\infty)$, is larger. In the instant before $t = \infty$, the distribution will be perfectly flat for $n \in [1, \infty)$ because $P_1 = P_2 = \cdots$ and therefore the distribution may have one mode value if $P_0(t \lesssim \infty) > P_n(t \lesssim \infty)$ is the greatest probability or an infinite number of mode values for each n if $P_n(t \lesssim \infty) > P_0(t \lesssim \infty)$ (this infinite-mode distribution is only possible if $P_0(t \lesssim \infty) \equiv 0$). The mean for a single chain, on the other hand, is $\overline{n}(t) = \mathrm{e}^{\alpha t}$ (we will derive this expression in the next section), which can take on any real value and is expected to go to 0 for $\alpha < 0$ or ∞ when $\alpha > 0$. Thus for a single chain, the mean and mode are almost always different quantities except in the infinite limit.

For the source distribution, the mean and mode may converge onto one another at any given time which is what we are witnessing as η transitions to values greater than 1. This is why η is referred to as the shape parameter in the last section of this chapter. Because of this source strength dependent convergence, the distribution will transition from the monotonically decreasing single-chain-like distribution (single chain physics dominates the distribution) to that of a unimodal distribution with $M(t) \sim \overline{n}(t)$.

Table 4.3: Associated data for the CDFs of Fig. 4.8.

η	S $[1/s]$	$\overline{n}(t=\tau)$
0.0001	$4.57 \cdot 10^5$	0.0076
1	$4.57 \cdot 10^9$	75.9
4	$1.83 \cdot 10^{10}$	303.5

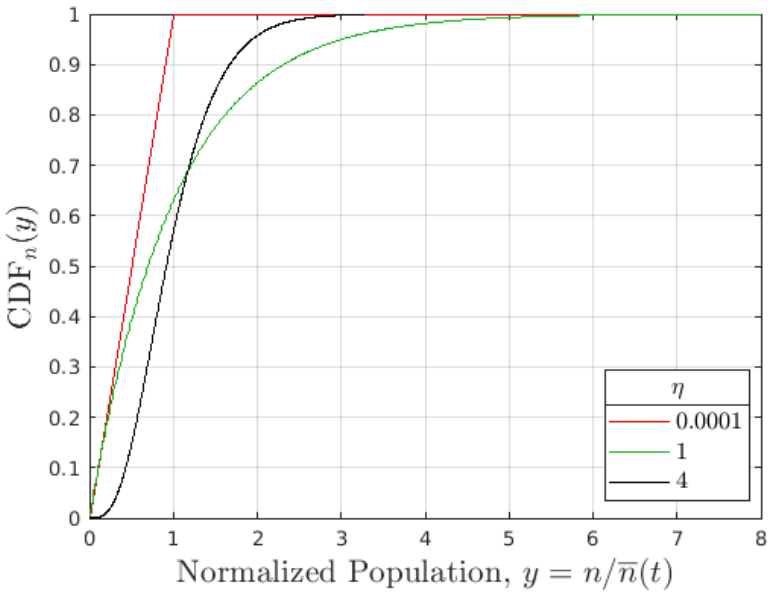


Figure 4.8: CDFs for several values of η compared against the average-normalized neutron population y. Here $k = 4.47$, $\tau = 1.85$ ns, and $t = \tau$.

approximated by the formula [40]:

$$C = \frac{10}{k-1}, \tag{4.134}$$

for $k > 1$. That is, as $k \to 1^+$, the likelihood of a single chain to diverge is less certain (than for larger k) and one must watch a chain for a longer time to guarantee divergence. As has been observed in practice by Gregson [31], one may set $C = 10^6$ for $k = 1.00001$, which may be regarded as the transition from a strongly stochastic to a weakly stochastic population regime for a single chain.

It is then a question of how large the neutron population must be with a source present, which is emitting single chains constantly and randomly, that the system becomes deterministic. It was suggested by Prinja & Souto that this transition can be assessed using the cumulative distribution function (CDF) about the mean, $\text{CDF}_n(\overline{n}(t)) = P(n \leq \overline{n}(t))$ where $\overline{n}(t)$ is the average population at time t and $P(n \leq \overline{n}(t))$ is read as the probability of n being less than or equal to $\overline{n}(t)$. The CDF

can be explicitly calculated as:

$$\begin{aligned}\mathrm{CDF}_n(\overline{n}(t)) &= \sum_{n=0}^{\lceil \overline{n}(t) \rceil} P_n(t) \\ &= \frac{1}{(1+b(t))^{\eta}\Gamma(\eta)} \sum_{n=0}^{\lceil \overline{n}(t) \rceil} \frac{\Gamma(\eta+n)}{n!} \left[\frac{b(t)}{1+b(t)}\right]^n\end{aligned} \tag{4.135}$$

where $\lceil \overline{n}(t) \rceil$ is the ceiling function for $\overline{n}(t)$ and $\overline{n}(t) = \frac{S}{\alpha}[\mathrm{e}^{\alpha t} - 1]$ for a source (derived in the next section). Figure 4.8 shows the CDF at a given time for varying source strengths as a function of the population normalized to the mean, $y(t) = n/\overline{n}(t)$. We see that a weak source for which $\eta = 0.0001$, the CDF very quickly goes to 1 before $y = 1$ which means the majority of the neutron population is less than the mean. For the case of a stronger source with $\eta = 4$, the CDF effectively goes from 0 to 1 at exactly $y = 1$. This tells us that the distribution is highly peaked and centered about the mean (the variance is low) and the population may be accurately represented by the mean. This latter characteristic is the hallmark of a deterministic system and thus the larger η is, the more centered about the mean the distribution is and the more accurate a deterministic model will be in predicting the behavior of the number distribution. An observation made by Hansen [29] suggests that we interpret η as being the expected number of persistent fission chains sponsored by a random but constant neutron source during the first e-folding time. Thus, as η increases, the number of persistent chains will also increase, pushing the population to larger numbers and decreasing the dispersion about the mean. On a final note, we mention that Prinja and Souto pointed out the quantity $y = n/\overline{n}(t)$ is a similarity variable for the distribution and therefore the CDFs of Fig. 4.8 will look the same regardless of the time.

Next we concern the asymptotic behavior of the distribution to understand the behavior of the survival probability and the POI in the presence of a source. Consider first the probability of there being zero neutrons at a given time, $P_0(t) = (1 + b(t))^{-\eta}$ (obtained by setting $n = 0$ in Eq. 4.61), and its limit (where we assume α is time-independent):

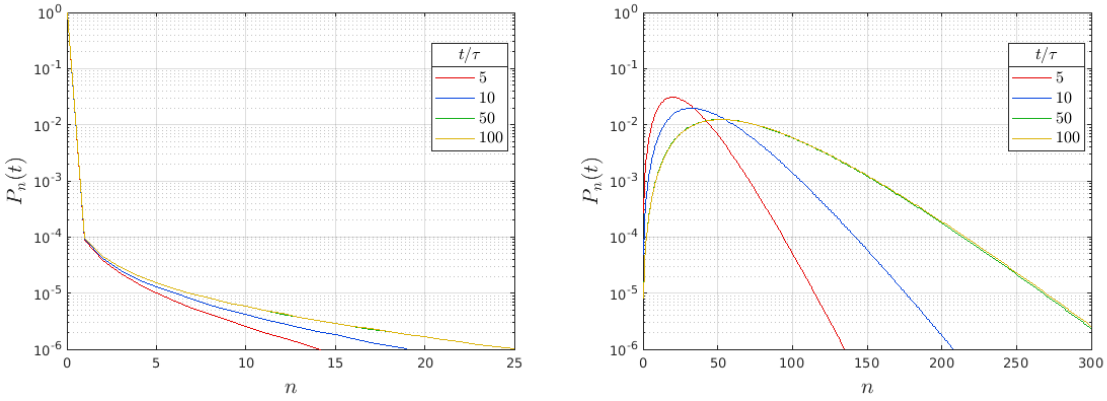
$$\lim_{t\to\infty} P_0(t) = \lim_{t\to\infty} \left[1 + \frac{\chi_2'}{2\alpha}\left[\mathrm{e}^{\alpha t} - 1\right]\right]^{-\eta} = \begin{cases} (1 + b_{\mathrm{sub}}(\infty))^{-\eta} & \text{if } \alpha < 0 \\ 0 & \text{if } \alpha > 0 \end{cases} \tag{4.136}$$

where $b_{\mathrm{sub}}(\infty) = \frac{\chi_2'}{2|\alpha|}$ is the limit of b in a subcritical system and $b_{\mathrm{super}}(\infty) = \infty$ is b for a supercritical system. This tells us that $P_0(\infty)$ approaches a constant value for subcritical systems while $P_0(\infty)$ vanishes for supercritical systems and the eventual extinction of the neutron population is impossible. Similarly, if we take the limit of the distribution for the remaining finite portion of the population, i.e. $n \in [1, \infty)$, we find:

$$\lim_{t\to\infty} P_n(t) = \frac{\Gamma(\eta+n)}{n!\Gamma(\eta)} \lim_{t\to\infty} \frac{1}{(1+b(t))^{\eta}} \cdot \frac{b(t)}{1+b(t)} = \begin{cases} \frac{1}{(1+b_{\mathrm{sub}}(\infty))^{\eta}} \frac{\Gamma(\eta+n)}{n!\Gamma(\eta)} \cdot \frac{b_{\mathrm{sub}}(\infty)}{1+b_{\mathrm{sub}}(\infty)} & \text{if } \alpha < 0 \\ 0 & \text{if } \alpha > 0 \end{cases} \tag{4.137}$$

Thus, we expect there to be a steady-state distribution for subcritical systems given by the top line of Eq. 4.137 (as opposed to the single chain subcritical case where the only possibility is a single non-zero probability at $n = 0$ with $P_0(\infty) = 1$). For a supercritical system, we once again find the $P_n(\infty)$ for all n goes to zero. By evoking the normalization condition, we find the POI for a supercritical system with a constant source:

$$P_{\infty}(\infty) = 1, \tag{4.138}$$



(a) **(b)**

Figure 4.9: Approach to steady-state for a subcritical system ($k = 0.90$) for (a) a weak source ($\eta = 0.0001$), and (b) a strong source ($\eta = 4$).

which tells us that a divergent chain is guaranteed to eventually emerge in a supercritical system.

On a final note, we consider a subcritical system of $k = 0.90$ at varying times for a weak source of $\eta = 0.0001$ ($S = 4.5 \cdot 10^5$ $1/s$), Fig. 4.9a, and a strong source of $\eta = 4$ (($S = 1.8 \cdot 10^{10}$ $1/s$)), Fig. 4.9b. Using the analysis for the single chain propagation, we know that the chains produced by either source eventually die off because $k < 1$. Although every chain is guaranteed to disappear, the distribution itself reaches a steady-state distribution and the number distribution becomes stationary (note the lines for $t = 50\tau$ and $t = 100\tau$ lie atop one another).

4.5 Moment Equations and the NMESA

Equations for the moments of the distribution are utilized for a myriad of applications, including, but not limited to: characterizing the number distribution for instances where the QA is not applicable; for fitting the distribution to another known distribution based on the calculated moments; or even for benchmarking codes. For illustrative purposes, we will show the general process for obtaining equations satisfied by the moments of the number distribution under investigation for the forward formulation, but any and all techniques presented are applicable in the backward formulation as well. We will demonstrate the NMESA by showing how to obtain ODEs satisfied by the moments of the distribution in Sec. 4.5.1 and then show how to use those moments to fit a distribution in Sec. 4.5.2.

4.5.1 Obtaining Moment Equations

To obtain the moments for the neutron number distribution from the forward master equation, Eq. 4.16, one would think to first apply the definition of the k^{th} moment of the population distribution,

$$\overline{n^k}(t) = \sum_{m=0}^{\infty} m^k P_m(t) \tag{4.139}$$

by multiplying by m^k and summing over all m. This methodology, albeit acceptable, is cumbersome as it would require one to perform the necessary transformations of the equation for every moment desired. Instead, by recognizing the similarity of Eq. 4.139 to the derivative of the PGF with respect to z evaluated at $z = 1$,

$$\begin{aligned}\left.\frac{\partial^k G(z,t)}{\partial z^k}\right|_{z=1} &= \left.\sum_{n=0}^{\infty} n(n-1)\cdots(n-k+1)z^{n-k}P_n(t)\right|_{z=1} \\ &= \overline{n(n-1)\cdots(n-k+1)}(t),\end{aligned} \tag{4.140}$$

we may systematically obtain the factorial moments to the distribution. In practice, this is done by taking derivatives with respect to z of the PGF PDE, Eq. 4.30, evaluating at $z = 1$, and unfolding the factorial moment expression to obtain $\overline{n^k}(t)$.

To begin, we state the forward PGF PDE:

$$\tau\frac{\partial G}{\partial t} = \left[-z + p_\ell + p_f g_{_f}(z)\right]\frac{\partial G}{\partial z} + S\tau\big[g_{_S}(z) - 1\big]G(z,t), \tag{4.141}$$

where we have written the reaction rates in terms of the average neutron lifetime, τ, and we have combined the capture and leakage into a single loss probability, $p_\ell = 1 - p_f$. By taking the derivative with respect to z of Eq. 4.141, we find:

$$\begin{aligned}\tau\frac{\partial^2 G}{\partial z\,\partial t} = &\left[-z + p_\ell + p_f g_{_f}(z)\right]\frac{\partial^2 G}{\partial z^2} + \left[-1 + p_f\frac{\mathrm{d}g_{_f}}{\mathrm{d}z}\right]\frac{\partial G}{\partial z} \\ &+ S\tau\big[g_{_S}(z) - 1\big]\frac{\partial G}{\partial z} + S\tau\frac{\mathrm{d}g_{_S}}{\mathrm{d}z}G,\end{aligned} \tag{4.142}$$

and upon evaluating at $z = 1$, we arrive at a linear first-order ordinary differential equation for the first moment of the neutron population:

$$\frac{\mathrm{d}\overline{n}(t)}{\mathrm{d}t} = \alpha(t)\,\overline{n}(t) + S(t)\overline{\nu}_{_S}, \tag{4.143}$$

which is the well-known point-reactor kinetic equation without delayed neutrons (as we mentioned in the introduction, master equations are called as such because all other equations describing the system can be derived from them- case-in-point Eq. 4.143). In Eq. 4.143, we are using $\alpha = (p_f\overline{\nu}_f - 1)/\tau = (k-1)/\tau$ and we have recognized $\mathrm{d}g_x/\,\mathrm{d}z|_{z=1} = \overline{\nu}_x$ provides the average of the specific multiplicity distribution, from which we may write the average of the factorial moments as

$$\begin{aligned}\left.\frac{\mathrm{d}^k g_x(z)}{\mathrm{d}z^k}\right|_{z=1} &= \overline{\nu_x(\nu_x-1)\cdots(\nu_x-k+1)} \\ &= \overline{(\nu_x)_k} \\ &= \chi_k\end{aligned} \tag{4.144}$$

where we are utilizing Pochhammer's notation for the falling factorial functions on the second line of the above and recall Eq. 4.38 for the last line. Equation 4.143 can be solved for using the integrating factor technique to yield:

$$\overline{n}(t) = \overline{n}(t_o)\mathrm{e}^{\int_{t_o}^{t}\mathrm{d}t'\alpha(t')} + \int_{t_o}^{t}\mathrm{d}t' S(t')\overline{\nu}_S \exp\left\{\int_{t'}^{t}\mathrm{d}t''\alpha(t'')\right\}, \tag{4.145}$$

which takes the form for constant α and S:

$$\overline{n}(t) = \overline{n}(0)\mathrm{e}^{\alpha(t-t_o)} + \frac{S\overline{\nu}_s}{\alpha}\left[\mathrm{e}^{\alpha(t-t_o)} - 1\right]. \tag{4.146}$$

For the single chain case, $\overline{n}(0) = 1$ and $S = 0$, while for the source case, $\overline{n}(0) = 0$, thus we have:

$$\text{Single Chain: } \overline{n}(t) = \mathrm{e}^{\alpha(t-t_o)} \tag{4.147a}$$

$$\text{Source: } \overline{n}(t) = \frac{S\overline{\nu}_s}{\alpha}\left[\mathrm{e}^{\alpha(t-t_o)} - 1\right]. \tag{4.147b}$$

We may obtain equations for the higher moments by taking successively higher derivatives of G. For the second moment, $\overline{n^2}(t)$, we have the linear first-order ODE that is coupled to the first moment:

$$\frac{\mathrm{d}\overline{n^2}(t)}{\mathrm{d}t} - 2\alpha(t)\overline{n^2}(t) = \frac{\mathrm{d}\overline{n}(t)}{\mathrm{d}t} + \left[\chi_2'(t) - 2\alpha(t) + 2S(t)\overline{\nu}_s\right]\overline{n}(t) + S(t)\overline{(\nu_s)}_2. \tag{4.148}$$

We see the RHS of the above is assumedly completely known as it is a function of $\overline{n}(t)$ and system parameters (λ_f, S). This ODE can be solved numerically, but we show how to obtain analytical solutions for constant system parameters. For the second moment, we find the solution using the integrating factor technique:

$$\begin{aligned}\overline{n^2}(t) =& \overline{n^2}(0)\mathrm{e}^{2\alpha t} + \int_0^t \mathrm{d}t' \frac{\mathrm{d}\overline{n}(t')}{\mathrm{d}t'}\mathrm{e}^{-2\alpha(t'-t)} + \frac{S\overline{\nu}_s}{\alpha}\left[\mathrm{e}^{2\alpha t} - 1\right] \\ &+ \left[\lambda_f\overline{(\nu_f)}_2 - 2\alpha + 2S\overline{\nu}_s\right]\int_0^t \mathrm{d}t'\overline{n}(t')\mathrm{e}^{-2\alpha(t'-t)}.\end{aligned} \tag{4.149}$$

This process must be applied as many times as there are desired moments. With some effort, it can be shown that for constant system parameters α and S, the k^{th} moment is:

$$\begin{aligned}\overline{n^k}(t) = \overline{n^k}(0)\mathrm{e}^{k\alpha t} + \frac{S\overline{(\nu_s)}_k}{k\alpha}\left[\mathrm{e}^{k\alpha t} - 1\right] + \sum_{j=1}^{k-1}\Bigg\{ &- s_1(k,j)\left[\overline{n^j}(t) - \overline{n^j}(0)\mathrm{e}^{k\alpha t}\right] \\ &+ c_j^{(k)}\int_0^t \mathrm{d}t'\overline{n^j}(t')\mathrm{e}^{-k\alpha(t'-t)}\Bigg\},\end{aligned} \tag{4.150}$$

where the coefficient is defined as:

$$c_j^{(k)} = \sum_{i=1}^{k-j} s_1(k-i,j)\left\{\binom{k}{i+1}\overline{(\nu_f)}_{i+1}\lambda_f + \binom{k}{i}\overline{(\nu_s)}_i S\right\}, \tag{4.151}$$

and s_1 is the Signed Stirling Number of the First Kind and $\binom{k}{j}$ is the binomial coefficient. Thus, to find the k^{th} moment of a number distribution, one must determine the $k-1$ lower moments.

4.5.2 Fitting a Distribution with the Moments

The primary reason for fitting a distribution using the moments is to circumvent the AMESA either because an analytical solution is unobtainable or because the NMESA is relatively easy to implement. Typically, the moment equations are not analytically solvable and must be solved numerically using

a discretization scheme. For brevity, we will avoid a conversation on the efficacy and performance of one numerical method over another, and will simply mention that we use MATLAB's intrinsic ODE solver, `ode45`, to numerically solve the system of ODEs Eqs. 4.143 and 4.148.

We will focus on constructing the neutron number distribution with a constant singlet-emitting source present, but we will also provide a single-chain expression for completeness. As proposed by Harris [20], and later verified and validated by Bell [9], the number distribution in the presence of a source asymptotically follows a gamma distribution when the neutron population has grown reasonably large ($\overline{n}(t) \gg 1$) and after several lifetimes ($t \gg 1/\alpha$- see footnote[3]). Bell found analytical solutions for the single chain and source distributions by assuming n was large enough within the system that it could be treated as a continuous variable. Thus he made the transition from a discrete probability distribution function to a probability density function: $P_n(t) \to P(n,t)\,\mathrm{d}n$. From there, he applied the inverse Laplace transform on G (Eqs. 4.47 and 4.53) and found the single chain and the source distributions:

$$\text{Single Chain: } P(n,t) = (1 - P_\infty(\infty))\,\delta(n) + \frac{[P_\infty(\infty)]^2}{\overline{n}(t)} \exp\left\{-\frac{P_\infty(\infty)}{\overline{n}(t)} n\right\} \tag{4.152a}$$

$$\text{Source: } P(n,t) = \left[\frac{\eta n}{\overline{n}(t)}\right]^{\eta-1} \frac{\eta}{\Gamma(\eta)\overline{n}(t)} \exp\left\{-\frac{\eta n}{\overline{n}(t)}\right\} \tag{4.152b}$$

where $\delta(n)$ is the Dirac delta function and we note that $P_\infty(\infty)$ in Eq. 4.152a is for a single chain (use Eq. 4.132), while $\eta = 2S/\chi_2'$ is Bell's parameter, $\overline{n}(t)$ is determined from Eq. 4.145 (single chain, set $S = 0$ and $\overline{n}(t_o) = 1$ and for the source case set $\overline{n}(t_o) = 0$), and $\Gamma(\cdot)$ is the gamma function. We note that the Prinja-Souto distributions given by Eqs. 4.57 (for the single chain) and 4.61 (for the source) are generalizations of Bell's distributions because they enforced n to remain a discrete variable. We wish to remind the reader that, when using Eqs. 4.152, $\alpha(t)$ can be time-dependent for both distributions while χ_2' can be time-dependent for the single chain case but must be held constant in the source case.

Henceforth, our discussion will concern only the source case. From this, we will follow suit with Harris and assume we may use a generic gamma distribution, $f(n;\theta,\beta)$, to model the number distribution, where n is a gamma-distributed random variable, θ is the shape parameter, and β is the rate parameter:

$$f(n;\theta,\beta) = \frac{\beta^\theta}{\Gamma(\theta)} n^{\theta-1} \mathrm{e}^{-\beta n}. \tag{4.153}$$

The mean and variance of the gamma distribution, μ_Γ and V_Γ, respectively, are given by:

$$\mu_\Gamma = \frac{\theta}{\beta} = \overline{n}(t) \tag{4.154a}$$

$$V_\Gamma = \frac{\theta}{\beta^2} = \frac{[\overline{n}(t)]^2}{\eta} \tag{4.154b}$$

Comparing Eq. 4.153 with Eq. 4.152b, we see that $\theta = \eta$ and $\beta = \eta/\overline{n}(t)$ to get the distributions to exactly match. However, we might be dealing with a system where the Quadratic Approximation does not hold or is not accurate whence Bell's distribution Eq. 4.152b and the Prinja-Souto distribution Eq. 4.61 fail. The primary regimes where these solutions fail are when the Quadratic Approximation is a poor approximation. This occurs for subcritical systems and for early times of

[3]Note that $\alpha = (k-1)/\tau$, which can be regarded as the excess neutron multiplication per neutron lifetime. Then the criteria $t \gg 1/\alpha$ is a requirement that enough time has passed such that the population is behaving in an asymptotic manner. The value of this criteria is system-dependent and is demonstrated below in Fig. 4.10.

supercritical systems for which the neutron population is still relatively small or when χ_2' is a strong function of time. We may then use the the generic gamma distribution Eq. 4.153 and calculate the two parameters θ and β to find an additional distribution. This will still be an approximation because the gamma distribution is not the exact representation of the neutron number distribution (case-in-point: the Prinja-Souto distribution is not a gamma distribution and it is more accurate than Bell's gamma distribution).

Proceeding, we may calculate the mean and variance using the first and second moment equations, Eqs. 4.143 and 4.148. These moment equations are not restricted by the QA and should provide more accurate results, numerical error notwithstanding, because we may use the entire multiplicity distribution as well as time-dependent system parameters (i.e., $\alpha(t)$ and $S(t)$). Thus, upon numerical calculation of the first and second moment, $\overline{n}_{_N}(t)$ and $\overline{n_{_N}^2}(t)$, where we use the subscript N to denote 'numerical', we may then calculate the true mean and variance of the neutron number distribution:

$$\mu_{_N}(t) = \overline{n}_{_N}(t) \tag{4.155a}$$

$$V_{_N}(t) = \overline{n_{_N}^2}(t) - \left[\overline{n}_{_N}(t)\right]^2. \tag{4.155b}$$

We relate this to the generic gamma distribution's parameters by setting $\mu_\Gamma = \mu_{_N}$ and $V_\Gamma = V_{_N}$ to find the relations:

$$\theta = \overline{n}_{_N}(t)\beta = \frac{\left[\mu_{_N}(t)\right]^2}{V_{_N}(t)} \tag{4.156a}$$

$$\beta = \frac{\mu_{_N}(t)}{V_{_N}(t)}. \tag{4.156b}$$

Finally, we make the observation that $\theta = \eta$ and $\beta = \eta/\overline{n}(t)$ and we are therefore tasked with calculating but a single fitting parameter, η_{fit} for Bell's distribution:

$$\eta_{\text{fit}}(t) = \theta = \frac{\left[\mu_{_N}(t)\right]^2}{V_{_N}(t)}. \tag{4.157}$$

The solution process is as follows:

1. calculate $\overline{n}_{_N}(t)$ and $\overline{n_{_N}^2}(t)$ from Eqs. 4.143 and 4.148,
2. calculate $\eta_{\text{fit}}(t)$ from Eq. 4.157 (alternatively calculate θ, β from Eqs. 4.156),
3. calculate the fitted distribution using $\overline{n}_{_N}(t)$ and $\eta_{\text{fit}}(t)$ in Eq. 4.152b (alternatively use θ, β in Eq. 4.153).

4.5.3 Comparing Source Distributions

We now compare distributions to gain an understanding of how the Bell and Prinja-Souto distributions are related and then demonstrate the gamma distribution fitting process as outlined above. We use MATLAB's intrinsic ODE solver, `ode45` to numerically solve the moment ODEs Eqs. 4.143 and 4.148 to complete steps 1 and 2 in the above list. The final step is to simply use those computed moments and parameters in Eq. 4.152b to find a distribution that (hopefully) resembles the neutron number distribution.

We first compare the Prinja-Souto distribution to the Bell distribution for subcritical and supercritical systems with a source present. Figure 4.10a shows a subcritical system with $k = 0.8788$; we see that both distributions asymptotically settle by 100 neutron lifetimes, but they do not converge

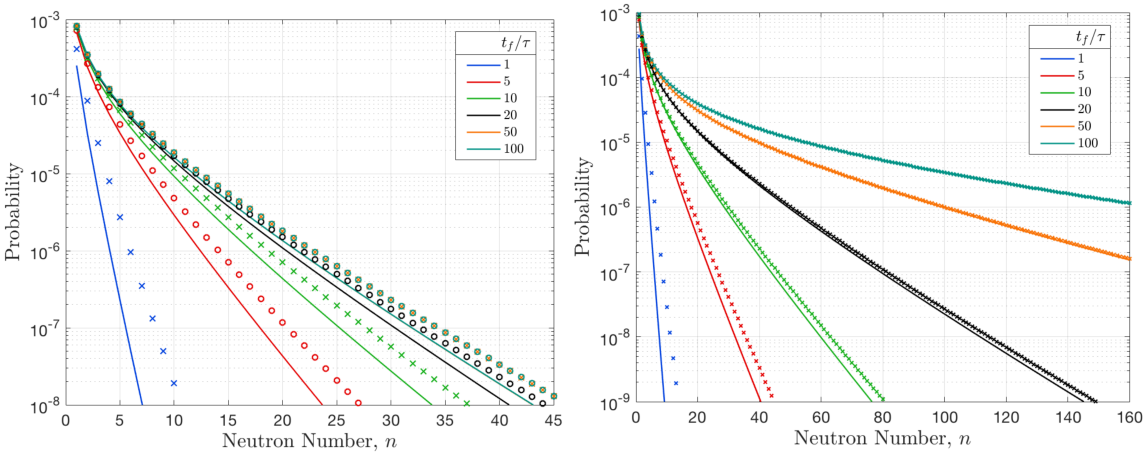


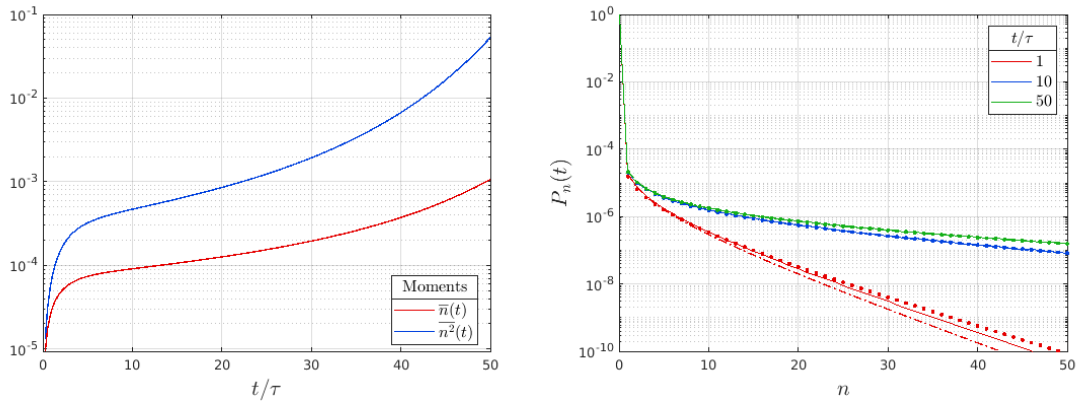
Figure 4.10: Comparison of the Bell and Prinja-Souto distributions for (a) a subcritical system and (b) a supercritical system with a source present. Solid lines are the Bell distribution and the discrete points, $\times$ and $\circ$, are the Prinja-Souto distribution.

Table 4.4: Initial fast neutron data for a ^{235}U metal system with time-dependent k and α.

$N\ [b^{-1}cm^{-1}]$	$\sigma_f\ [b]$	$\sigma_c\ [b]$	$v\ [cm/s]$	$\tau\ [ns]$	$\chi_2'\ [1/s]$
0.05088	2.053	8.109	$5.174 \cdot 10^9$	0.374	$9.144 \cdot 10^9$
t_o	t_f	k_o	k_f	$\alpha_o\ [1/s]$	$\gamma\ [ns]$
0	50τ	0.5	1.1	$-1.34 \cdot 10^9$	2.41

onto one another. Thus, the distributions for subcritical systems do not share an asymptotic form. This tells us that Bell's distribution should not be applied to subcritical systems for $k < 0.9$, except to determine a very crude estimate of the number distribution. However, the supercritical system of Fig. 4.10b, with $k = 1.0035$, shows that the discrete and continuous distributions do indeed converge to a common form. Then it can be said that Bell's distribution is applicable for marginally supercritical systems after several decades of neutron lifetimes. This is an important point to keep in mind when attempting to fit a gamma distribution using the moments because it might not be representative of the *actual* number distribution. A researcher must remain skeptical of results, especially when making approximations in the realm of stochastic neutronics. We note in passing that the best benchmark to obtain number distributions is by use of Monte Carlo methods which tend to be very time-consuming and computationally expensive calculations, but the actual distribution is more than likely guaranteed through such methods. We will learn about Monte Carlo methods in a later primer volume.

We now turn our focus to solving the moment equations for a system with a constant singlet-emitting source and we allow for a linearly varying criticality $k(t)$ (and thus linear $\alpha(t)$). For a system with an initial multiplication factor k_o at time t_o that is then subject to a linear change over



(a) **(b)**

Figure 4.11: (a) Moments and (b) number distributions at differing times of the system evolution for a system with a linearly varying $\alpha(t)$ and a weak source of $S = 10^5\ 1/s$ ($\eta = 2.1872 \cdot 10^{-5}$). In (b), the dots correspond to the fitted distribution, solid lines are the Prinja-Souto distribution (Eq. 4.61), and dashed lines are Bell's distribution (Eq. 4.152b).

time, we have:

$$k(t) = k_o + \frac{\Delta k}{\Delta t}(t - t_o), \tag{4.158}$$

where $\Delta k = k_f - k_o$, $\Delta t = t_f - t_o$, and k_f is the criticality at some prescribed final time t_f. We additionally have

$$\alpha(t) = \frac{k(t) - 1}{\tau} = \frac{\Delta k(t - t_o)}{\tau \Delta t} + \alpha_o, \tag{4.159}$$

where $\alpha_o = (k_o - 1)/\tau$ and we are assuming that τ is constant. Equations 4.44 may be computed:

$$a(t) = \exp\left\{\frac{t^2 - 2tt_o + t_o^2}{4\gamma^2} + \alpha_o(t - t_o)\right\} \tag{4.160a}$$

$$b(t) = ca(t)\left[\text{erf}\left(\gamma\alpha(t)\right) - \text{erf}\left(\gamma\alpha_o\right)\right] \tag{4.160b}$$

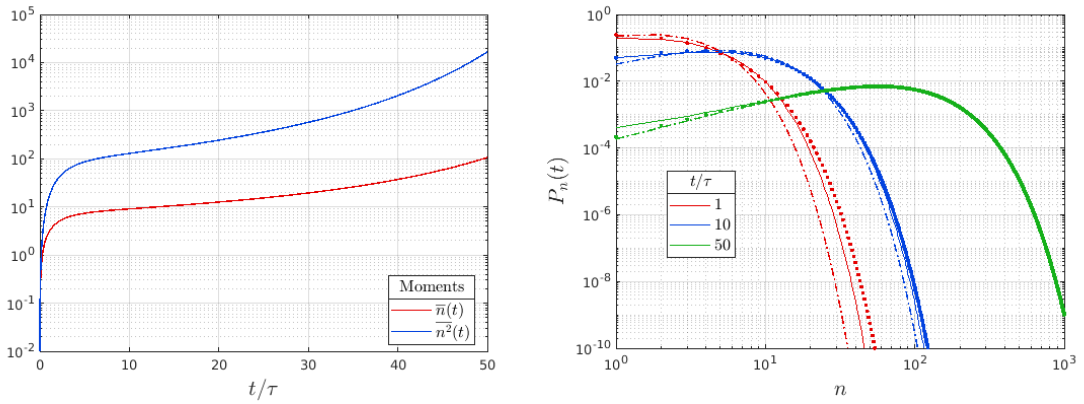
$$c = \frac{\chi_2'}{2}\sqrt{\pi}\,\gamma \text{e}^{(\gamma\alpha_o)^2} \tag{4.160c}$$

$$\gamma = \sqrt{\frac{\tau}{2}\frac{\Delta t}{\Delta k}} \tag{4.160d}$$

where we have assumed χ_2' is constant (therefore λ_f is constant) and $\text{erf}(\cdot)$ is the error function. From this, we may compute the single chain survival probability $P_S(t) = a(t)/(1 + b(t))$ and the single chain POI is then (using Eq. 4.132):

$$P_\infty(\infty) = \frac{1}{c\left[1 - \text{erf}\left(\gamma\alpha_o\right)\right]}. \tag{4.161}$$

Consider now the ^{235}U system from before using fast neutron multiplicity data from Table 4.1 as well as the data in Table 4.4 for the initial system data. The system begins at a very low subcritical state of $k_o = 0.5$ and reaches a value of $k_f = 1.1$ at a time of $t_f = 50\tau$. Thus, using Eq.



(a) **(b)**

Figure 4.12: Per Fig. 4.11, but for a strong source of $S = 10^{10}$ $1/s$ ($\eta = 2.1872$).

4.158, the system is subcritical until about $t \approx 41.667\tau$, at which time it becomes increasingly more supercritical. We show in Fig. 4.11a the numerically computed moment ODEs for the case in which the system possesses a weak neutron source of $S = 10^5$ $1/s$ (thus $\eta = 2.1872 \cdot 10^{-5}$) over the range of 50τ. The mean is increasing in the subcritical time range $t < 41.7\tau$ because the multiplication is increasing, thus the mean will be higher for higher k even in steady-state. Figure 4.11b provides the number distribution at different times of this evolutionary process as calculated by the gamma distribution fitting method (dots), the analytical Prinja-Souto distribution (solid lines) using Eq. 4.61, and Bell's distribution (dashed lines) using Eq. 4.152b. Note that we used the numerically calculated $\overline{n}(t)$ in Bell's distribution (and, just to be clear, we use $\eta = 2S/\chi_2'$, not Eq. 4.157). All three distributions agree by $t = 50\tau$, where we note that the fitted distribution better approximates the Prinja-Souto distribution than the Bell distribution does at $t = \tau$. This suggests that one may be more inclined to use the fitted distribution over Bell's distribution to better model the number distribution at early times.

Next, we increase the source strength by 5 orders of magnitude to $S = 10^{10}$ $1/s$ and display the results in Figs. 4.12b. We see the moments have the same shape as in the weak source case, but are, as expected, drastically larger in magnitude. Figure 4.12 shows the three number distributions once again where the distributions are now unimodal due to $\eta > 1$. As with Fig. 4.11b, we see the fitted distribution agrees with the Prinja-Souto distribution earlier by around $t = 10\tau$ and all distributions agree by $t = 50\tau$. Therefore a main result from this study is that the gamma distribution fitting works well for strong and weak sources (i.e., is well-suited for both the monotonically decreasing form as well as the unimodal form) in both sub- and supercritical systems after only a few neutron lifetimes (this is because the distributions agree for $t = 10\tau$ when the system is still quite subcritical with $k(10\tau) = 0.62$). We again wish to express caution in interpreting the overall accuracy and precision of these results because both the Bell and Prinja-Souto distributions rely on the Quadratic Approximation and are therefore approximate distributions with specific domains of validity. We intentionally avoided a conversation about Monte Carlo methods, which tend to provide the most accurate and general results (given appropriate statistical convergence and proper simulation of the physics), to maintain an analytical focus to this primer and this will be a topic for the next volume.

A final observation concerns the mean between the two different source strengths of Figs. 4.11a and 4.12a. Note the similarity between final mean values, $\overline{n}_{\text{weak}}(50\tau) = 10^{-3}$ neutrons and

$\overline{n}_{\text{strong}}(50\tau) = 10^2$ neutrons, and the source magnitudes $S_{\text{weak}} = 10^5$ $1/s$ and $S_{\text{strong}} = 10^{10}$ $1/s$. The difference in magnitude between both quantities, 10^5, is the same. This is not a coincidence as this holds for all time in this problem and indeed for all problems as it is a scaling symmetry commonly exploited in the literature and in practice. This scaling can be seen in Eq. 4.145, or more clearly in Eq. 4.147b, where the solution $\overline{n}(t)$ is directly proportional to the source strength. This brings us to our final point, concerning the approximation of singlet-emitting sources. As can be seen in Eq. 4.145 (or 4.147b), the solution is actually directly proportional to the product $S\overline{\nu}_S$, where $\overline{\nu}_S = 1$ for a singlet-emitting source. We can therefore increase S by a factor of $\overline{\nu}_S$ to determine the mean at a given time rather than re-do the calculation at every time-step. Similarly, we may alter Bell's parameter $\eta = 2S/\chi_2'$ by a factor $\overline{\nu}_S$ to accordingly adjust the number distribution for non-singlet-emitting sources.

Chapter 5

Conclusions

This primer was motivated towards teaching the fundamental principles of stochastic neutronics and to use those principles to model systems of interest. We demonstrated the Master Equation Solution Algorithm in chapters 2, 3, and 4 for both the Forward Formulation and the Backward Formulation. For chapters 2 and 3, we obtained exact analytical solutions for the Radioactive Decay Model and the Binary Fission Model without capture, respectively, due to the simplicity of the models. Chapter 4, which concerned a full neutron multiplicity distribution for the induced fission and spontaneous fission, required the application of the Quadratic Approximation to obtain an analytical solution for the single chain number distribution and we further required constant χ_2' and singlet-emitting sources to obtain an analytical expression for the source number distribution. We hope that the reader emerges at the end of their reading this primer with the core concepts understood insofar that they may go on to derive and solve their own Master equations in their fields of study.

Though there are many places to turn to next, we recommend reading the many-times mentioned papers by Bell [9] and Prinja & Souto [16] for their own commentary, derivations, and insights. These two papers utilize the forward formulation while Bell's paper includes delayed neutrons, a detailed analysis of the characteristic curves of G and z, and a derivation of the distributions that are his namesake. The Prinja-Souto distribution does not have delayed neutrons but it succeeds in its goal of deriving the generalized number distributions that we call to throughout Chapter 4. They provide the analysis we used to understand the asymptotic distributions and they provide proof that their distributions converge to Bell's distributions. The reader is referred to Prinja's paper [18] for the zero-dimensional backward formulation to the stochastic neutronics equations seen in Chapter 4 with additional discussion on the survival probability.

A list of other papers with generalizations is provided now for the committed reader, and we will plan on addressing many of these generalizations in later primer volumes. An additional resource includes Pázsit and Pál's text [7] to experience the many applications and generalizations of the models we discussed herein. For generalizations of the stochastic model discussed herein, Pàl [22, 23], Bell [21], and Lewins [24] provide the backward formulation with space, angle, and energy effects, while the forward formulation with phase-space is provided by Stacey [25]. Delayed neutrons are considered in Bell [9] (although no analytical solution is found,) and Muñoz-Cobo provides phase-space equations with delayed neutrons [34]. Additional particle species are incorporated in works such as photon-neutron coupling and counting statistics [33, 35, 36, 6, 37], fission numbers [26], and fission energy deposition [27, 28]. To gain insight on experimental results and understanding of stochastic neutronics, the reader is referred to a few useful documents here: [29, 30, 31, 32], though there are many others. We mention these generalizations of the stochastic theory of neutron

transport to provide scope, context, applications, and once again, to signify that this work is only the first step within the problem space of stochastic neutronics. In future volumes, we will be applying generalizations to the models, such as space- and angle-dependence and providing more examples to help cultivate a deeper understanding of stochastic neutron populations within multiplying systems.

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